1239344

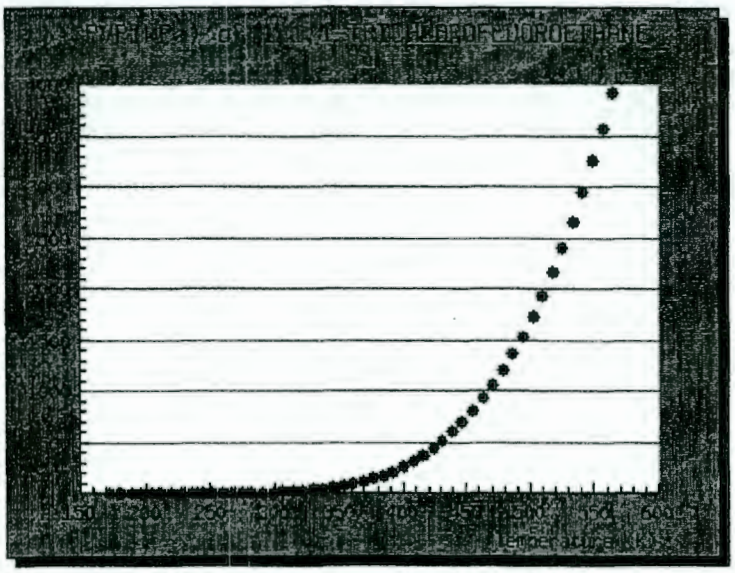
CLASS 1 MODIFICATIONS TO HANFORD FACILITY RCRA PERMIT

SECTION 5 OF 7

Temperature Dependent Properties

CAS: 27154-33-2

[PVP] Vapor pressure of 1,1,1-TRICHLOROFLUOROETHANE



Equation Name	KDB Correlation Equation	
Equation	ln(Pvp) = A*ln(T) + B/T + C + D*T^2 where Pvp in kPa, T in K	
Coefficient A	-5.953147E+00	
Coefficient B	-5.846863E+03	
Coefficient C	5.526425E+01	
Coefficient D	3.384266E-06	
Coefficient E		
Coefficient F		
Coefficient G		
T range , from	173.00	K
T range , to	565.00	K

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000506-68-3
Chem Name  : CYANOGEN BROMIDE
Mol Formula: CBrN
Mol Weight : 105.93
Melting Pt : 52 deg C
Boiling Pt : 61.5 deg C
Water Solubility:
   Value : 1.08E+005 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : -0.29
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 122 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : OHE,S (1976)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000506-77-4 Name: CYANOGEN CHLORIDE

```
*******************************************************************************
VP      CYANOGEN CHLORIDE                                        CAS#   506-77-4
  Vapor Pressure :  1.225E+03   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000506-77-4
Chem Name  : CYANOGEN CHLORIDE
Mol Formula: CClN
Mol Weight : 61.47
Melting Pt : -6.5 deg C
Boiling Pt : 13 deg C
Water Solubility:
   Value : 6E+004 mg/L
   Temp  : 0 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : -0.38
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 1230 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0245 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000540-59-0 Name: 1,2-DICHLOROETHYLENE

```
*******************************************************************************
MELT    1,2-DICHLOROETHYLENE                                    CAS#   540-59-0
  Melting Point  :  -57          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*******************************************************************************

VP      1,2-DICHLOROETHYLENE                                    CAS#   540-59-0
  Vapor Pressure :  201-331      MM HG
  Temperature (C):  25
  Remarks        :  RANGE DEFINED BY VALUES FOR CIS & TRANS ISOMERS, SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************
```

ALDRICH (1988)
ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI: ALDRICH CHEM CO.; 1988

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dichloropropene, 1,3-
CAS Number: 000542-75-6

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	3.0E-2	mg/kg/day	IRIS
Inhal RfD:	5.7E-3	mg/kg/day	IRIS
Oral Slope:	1.0E-1	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	1.4E-2	(mg/kg/day)^-1	HEAST
Inhal Wt-of-Evid:	B2		
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	4.7E+2	mg/kg	ACGIH
Dermal LD50:	5.0E+2	mg/kg	ACGIH
Gas Inhal LC50:	1.0E+3	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.1E+2	µg/L	ECOTOX
Salt Ecol LC50:	7.0E+2	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.1E+1	days	FATERATE
Volatility:	9.3E+1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.1E+1	days	FATERATE
Volatility:	1.0E+0	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
Log Kow:	1.6E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.1E+2	
Density:	1.2E+0	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	3.4E+1	Torr	CHEMFATE
Henry's Law:	1.8E-2	atm-m3/mol	CHEMFATE
Water Solub:	2.8E+3	mg/L	CHEMFATE
Distrib Coef:	9.1E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.6E+0		CHEMFATE
Water Solub:	2.8E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:		C
Boiling Point:	1.1E+2	C
Formula:	C3 H4 Cl2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000542-75-6 Name: 1,3-DICHLOROPROPYLENE

```
*******************************************************************************
MELT     1,3-DICHLOROPROPYLENE                                  CAS#   542-75-6
  Melting Point  :  -48          DEGC
  Remarks        :  ESTIMATED BY EQUATION 20 IN NEELY,WB & BLAU,GE (1985), SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP       1,3-DICHLOROPROPYLENE                                  CAS#   542-75-6
  Vapor Pressure :  34           MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DILLING,WL (1977)
*******************************************************************************
```

DILLING,WL (1977)
DILLING,W.L.; INTERPHASE TRANSFER PROCESSES. II. EVAPORATION RATES OF CHLOROMETHANES, ETHANES, ETHYLENES, PROPANES, AND PROPYLENES FROM DILUTE AQUEOUS SOLUTIONS. COMPARISONS WITH THEORETICAL PREDICTIONS.; ENVIRON. SCI. TECHNOL.; 11:405-9.; 1977

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Carbon tetrachloride

CAS Number: 000056-23-5

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	7.0E-4	mg/kg/day	IRIS
Inhal RfD:	5.7E-3	mg/kg/day	STSC
Oral Slope:	1.3E-1	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	5.2E-2	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	B2		
Oral ED10:	1.7E-2	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	1.7E-2	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	2.3E+3	mg/kg	ACGIH
Dermal LD50:	1.5E+4	mg/kg	ACGIH
Gas Inhal LC50:	7.3E+3	ppm	ACGIH
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.0E+3	µg/L	ECOTOX
Salt Ecol LC50:	5.0E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	2.6E+6	days	CHEMFATE
Volatility:	1.1E+2	days	THOMAS
Photolysis:	1.1E+3	days	CHEMFATE
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	2.6E+6	days	CHEMFATE
Volatility:	1.2E+0	days	THOMAS
Photolysis:	1.1E+3	days	CHEMFATE
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
Log Kow:	2.8E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.5E+2	
Density:	1.6E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.2E+2	Torr	CHEMFATE
Henry's Law:	3.0E-2	atm-m3/mol	CHEMFATE
Water Solub:	7.9E+2	mg/L	CHEMFATE
Distrib Coef:	3.5E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	3.0E+1		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	3.0E+2		ECOTOX
Salt BCF:			
Log Kow:	2.8E+0		CHEMFATE
Water Solub:	7.9E+2		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-2.3E+1	C
Boiling Point:	7.7E+1	C
Formula:	C Cl4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000056-23-5 Name: CARBON TETRACHLORIDE

```
*******************************************************************************
MELT     CARBON TETRACHLORIDE                                    CAS#     56-23-5
  Melting Point  :  -23          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP       CARBON TETRACHLORIDE                                    CAS#     56-23-5
  Vapor Pressure :  .115E 03     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  FROM JOHN,R. (1976)
  Abbrev. Ref.   :  ROGERS,RD & MCFARLANE,JC (1981)
*******************************************************************************

VP       CARBON TETRACHLORIDE                                    CAS#     56-23-5
  Vapor Pressure :  .5200E+02    .1090E+03    .1990E+03   TORR        MEASURED
  Temperature (C):  10.0         25.0         40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1966B)
*******************************************************************************

VP       CARBON TETRACHLORIDE                                    CAS#     56-23-5
  Vapor Pressure :  115          MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP       CARBON TETRACHLORIDE                                    CAS#     56-23-5
  Vapor Pressure :  114          MM HG        MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA,

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

GALLANT,RW (1966B)
GALLANT,R.W.; PHYSICAL PROPERTIES OF HYDROCARBONS. V. CHLORINATED METHANES. HYDROCARBON PROCESS.; 45:161-9.; 1966B

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

ROGERS,RD & MCFARLANE,JC (1981)
ROGERS,R.D.; MCFARLANE,J.C.; SORPTION OF CARBON TETRACHLORIDE, ETHYLENE DIBROMIDE AND TRICHLOROETHYLENE IN SOIL AND CLAY.; ENVIRON. MONIT. ASSESS.; 1:155-8.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000593-60-2 Name: BROMOETHYLENE

```
*******************************************************************************
MELT    BROMOETHYLENE                                          CAS#   593-60-2
  Melting Point  :  -139.54     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC (1972)
*******************************************************************************

VP      BROMOETHYLENE                                          CAS#   593-60-2
  Vapor Pressure :  1033        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************
```

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

WEAST,RC (1972)
WEAST,R.C.; HANDBOOK OF CHEMISTRY AND PHYSICS, 53RD ED.; CLEVELAND, OH: TH CHEMICAL RUBBER COMPANY.; 1972

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000630-20-6 Name: 1,1,1,2-TETRACHLOROETHANE

```
*******************************************************************************
MELT    1,1,1,2-TETRACHLOROETHANE                          CAS#   630-20-6
  Melting Point  :  -68.7       DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ARCHER,WL (1979)
*******************************************************************************

VP      1,1,1,2-TETRACHLOROETHANE                          CAS#   630-20-6
  Vapor Pressure :  12.03       MM HG       CALC
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM TEMP RANGE 59.3-130.2 DEG C
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1,1,1,2-TETRACHLOROETHANE                          CAS#   630-20-6
  Vapor Pressure :  1.203E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

ARCHER,WL (1979)
ARCHER,W.L.; OTHER CHLOROETHANES.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 5:722-42.; 1979

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Chloroform

CAS Number: 000067-66-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	1.0E-2	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:	8.1E-2	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	B2		
Oral ED10:	5.1E-1	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	5.1E-1	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	3.6E+1	mg/kg	RTECS
Dermal LD50:	2.0E+4	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:	4.9E+4	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	8.5E+3	µg/L	ECOTOX
Salt Ecol LC50:	2.8E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.3E+6	days	CHEMFATE
Volatility:	9.6E+1	days	THOMAS
Photolysis:	1.6E+2	days	CHEMFATE
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.3E+6	days	CHEMFATE
Volatility:	1.0E+0	days	THOMAS
Photolysis:	1.6E+2	days	CHEMFATE
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.0E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.2E+2	
Density:	1.5E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.0E+2	Torr	CHEMFATE
Henry's Law:	3.7E-3	atm-m3/mol	CHEMFATE
Water Solub:	7.9E+3	mg/L	CHEMFATE
Distrib Coef:	8.0E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	6.0E+0		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	6.9E+2		ECOTOX
Salt BCF:			
Log Kow:	2.0E+0		CHEMFATE
Water Solub:	7.9E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-6.4E+1	C
Boiling Point:	6.1E+1	C
Formula:	C H Cl3	

CLASS INFORMATION

Class	Parent Substance

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CHEMFATE Search Results

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CAS #: 000067-66-3 Name: CHLOROFORM

```
*****************************************************************************
MELT    CHLOROFORM                                          CAS#    67-66-3
  Melting Point  :  -63.52      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      CHLOROFORM                                          CAS#    67-66-3
  Vapor Pressure :  .9700E+02   .2460E+03   .3620E+03   TORR        MEASURED
  Temperature (C):  10.0        25.0        40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1966B)
*****************************************************************************

VP      CHLOROFORM                                          CAS#    67-66-3
  Vapor Pressure :  .200E 03    TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  THIBODEAUX,LJ (1981)
*****************************************************************************

VP      CHLOROFORM                                          CAS#    67-66-3
  Vapor Pressure :  197         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************

VP      CHLOROFORM                                          CAS#    67-66-3
  Vapor Pressure :  197.3       MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

GALLANT,RW (1966B)
GALLANT,R.W.; PHYSICAL PROPERTIES OF HYDROCARBONS. V. CHLORINATED METHANES. HYDROCARBON PROCESS.; 45:161-9.; 1966B

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THIBODEAUX,L.J.; ESTIMATING THE AIR EMISSIONS OF CHEMICALS FROM HAZARDOUS WASTE LANDFILLS.; J. HAZARDOUS MATERIALS; 4:235-44.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000684-16-2 Name: HEXAFLUORO-2-PROPANONE

```
*******************************************************************************
VP      HEXAFLUORO-2-PROPANONE                                  CAS#   684-16-2
  Vapor Pressure :  5.000E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000684-16-2
Chem Name  : HEXAFLUORO-2-PROPANONE
Mol Formula: C3F6O
Mol Weight : 166.02
Melting Pt : -125 deg C
Boiling Pt : -27.4 deg C
Water Solubility:
   Value : 3640 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 1.46
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 2230 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.00307 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trichloroethane, 1,1,1-
CAS Number: 000071-55-6

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:	6.3E-1	mg/kg/day	STSC
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	5.7E+3	mg/kg	ACGIH
Dermal LD50:	1.6E+4	mg/kg	ACGIH
Gas Inhal LC50:	3.9E+3	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	3.5E+4	µg/L	ECOTOX
Salt Ecol LC50:	3.1E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.8E+2	days	CHEMFATE
Volatility:	1.0E+2	days	THOMAS
Photolysis:		days	
Biodeg:	2.7E+2	days	CHEMFATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.8E+2	days	CHEMFATE
Volatility:	1.1E+0	days	THOMAS
Photolysis:		days	
Biodeg:	2.7E+2	days	CHEMFATE
Radio:		days	
Log Kow:	2.5E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.3E+2	
Density:	1.3E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.2E+2	Torr	CHEMFATE
Henry's Law:	1.7E-2	atm-m3/mol	CHEMFATE
Water Solub:	1.3E+3	mg/L	CHEMFATE
Distrib Coef:	2.2E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	9.0E+0		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	9.0E+0		ECOTOX
Salt BCF:			
Log Kow:	2.5E+0		CHEMFATE
Water Solub:	1.3E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-3.0E+1	C
Boiling Point:	7.4E+1	C
Formula:	C2 H3 Cl3	

CLASS INFORMATION

Class	Parent Substance

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000071-55-6 Name: 1,1,1-TRICHLOROETHANE

```
*******************************************************************************
MELT    1,1,1-TRICHLOROETHANE                                   CAS#    71-55-6
  Melting Point  :  -30.4        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      1,1,1-TRICHLOROETHANE                                   CAS#    71-55-6
  Vapor Pressure :  .1000E+03    .2380E+03    TORR        MEASURED
  Temperature (C):  20.0         40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  ARCHER,WL (1979)
*******************************************************************************

VP      1,1,1-TRICHLOROETHANE                                   CAS#    71-55-6
  Vapor Pressure :  124          MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1,1,1-TRICHLOROETHANE                                   CAS#    71-55-6
  Vapor Pressure :  123.733      MM HG        MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

ARCHER,WL (1979)
ARCHER,W.L.; OTHER CHLOROETHANES.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 5:722-42.; 1979

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000074-83-9 Name: METHYL BROMIDE

```
*******************************************************************************
MELT    METHYL BROMIDE                                          CAS#    74-83-9
  Melting Point  :  -94.07      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      METHYL BROMIDE                                          CAS#    74-83-9
  Vapor Pressure :  .1400E 04   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  NEELY,WB (1976)
*******************************************************************************

VP      METHYL BROMIDE                                          CAS#    74-83-9
  Vapor Pressure :  .9495E 03   .1615E 04   TORR        MEASURED
  Temperature (C):  10.         25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  DAELEMANS,A & SIEBERING,H (1977)
*******************************************************************************

VP      METHYL BROMIDE                                          CAS#    74-83-9
  Vapor Pressure :  1616        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAELEMANS,A & SIEBERING,H (1977)
DAELEMANS,A.; SIEBERING,H.; DISTRIBUTION OF METHYL BROMIDE OVER THE PHASES SOIL.; MEDED. FAC. LANDBOUWWET., RIJKSUNIV. GENT.; 42:1729-38.; 1977

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NEELY,WB (1976)
NEELY,W.B.; PREDICTING THE FLUX OF ORGANICS ACROSS THE AIR/WATER INTERFACE. CONTROL HAZARD MATER. SPILLS, PROC. NAT. CONF. 3RD. PP 197-200.; 1976

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CAS #: 000074-87-3 Name: METHYL CHLORIDE

```
*******************************************************************************
MELT     METHYL CHLORIDE                                          CAS#     74-87-3
  Melting Point  :  -97.70       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP       METHYL CHLORIDE                                          CAS#     74-87-3
  Vapor Pressure :  .1918E 04    .3670E 04    .6387E 04    TORR        MEASURED
  Temperature (C):  0.           20.          40.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AHLSTROM,RCJR & STEELE,JM (1979)
*******************************************************************************

VP       METHYL CHLORIDE                                          CAS#     74-87-3
  Vapor Pressure :  4300         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

AHLSTROM,RCJR & STEELE,JM (1979)
AHLSTROM,R.C. JR.; STEELE,J.M.; METHYL CHLORIDE.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 5:677-85.; 1979

DAUBERT,TE & DANNER,RP (1985)
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RIDDICK,JA ET AL. (1986)
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End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000074-88-4 Name: METHYL IODIDE

```
*******************************************************************************
MELT    METHYL IODIDE                                          CAS#    74-88-4
  Melting Point  :  -66.45      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      METHYL IODIDE                                          CAS#    74-88-4
  Vapor Pressure :  405         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      METHYL IODIDE                                          CAS#    74-88-4
  Vapor Pressure :  404.46      MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000074-95-3 Name: DIBROMOMETHANE

```
*******************************************************************************
MELT    DIBROMOMETHANE                                          CAS#    74-95-3
  Melting Point  :  -52.7       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      DIBROMOMETHANE                                          CAS#    74-95-3
  Vapor Pressure :  44.4        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KUDCHADKER,AP ET AL. (1979)
*******************************************************************************
```

KUDCHADKER,AP ET AL. (1979)
KUDCHADKER,A.P.; KUDCHADKER,S.A.; SHUKLA,R.P.; PATNAIK,P.R.; VAPOR PRESSURE AND BOILING POINTS OD SELECTED HALOMETHANES.; J. PHYS. CHEM. REF. DATA.; 8:499-517.; 1979

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MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000074-97-5
Chem Name  : CHLOROBROMOMETHANE
Mol Formula: CH2BrCl
Mol Weight : 129.38
Melting Pt : -87.9 deg C
Boiling Pt : 68 deg C
Water Solubility:
   Value : 1.67E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.41
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 143 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.00146 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 8.8E-014 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DEMORE,WB (1996)
```

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SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Ethyl chloride

CAS Number: 000075-00-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:	2.9E+0	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:	6.1E+4	ppm	ACGIH
Dust Inhal LC50:	1.2E+5	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.8E+1	days	FATERATE
Volatility:	1.8E-1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.8E+1	days	FATERATE
Volatility:	1.8E-1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
Log Kow:	1.4E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	6.5E+1	
Density:	8.9E-1	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.0E+3	Torr	CHEMFATE
Henry's Law:	8.8E-3	atm-m3/mol	CHEMFATE
Water Solub:	5.7E+3	mg/L	CHEMFATE
Distrib Coef:	3.2E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.4E+0		CHEMFATE
Water Solub:	5.7E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.4E+2	C
Boiling Point:	1.2E+1	C
Formula:	C2 H5 Cl	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-00-3 Name: CHLOROETHANE

```
*******************************************************************************
MELT    CHLOROETHANE                                          CAS#    75-00-3
  Melting Point  :  -136.4      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      CHLOROETHANE                                          CAS#    75-00-3
  Vapor Pressure :  1008        MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Vinyl chloride
CAS Number: 000075-01-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	3.0E-3	mg/kg/day	IRIS
Inhal RfD:	2.9E-2	mg/kg/day	IRIS
Oral Slope:	1.5E+0	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	A		
Inhal Slope:	3.1E-2	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	A		
Oral ED10:	5.5E-2	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	A		
Inhal ED10:	5.5E-2	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	A		
Oral LD50:	5.0E+2	mg/kg	RTECS
Dermal LD50:		mg/kg	
Gas Inhal LC50:	1.8E+1	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.7E-1	days	THOMAS
Photolysis:	7.5E-1	days	CHEMFATE
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.7E-1	days	THOMAS
Photolysis:	7.5E-1	days	CHEMFATE
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	1.4E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	6.3E+1	
Density:	9.1E-1	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	3.0E+3	Torr	CHEMFATE
Henry's Law:	2.7E-2	atm-m3/mol	CHEMFATE
Water Solub:	8.8E+3	mg/L	CHEMFATE
Distrib Coef:	3.7E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.4E+0		CHEMFATE
Water Solub:	8.8E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.5E+2	C
Boiling Point:	-1.3E+1	C
Formula:	C2 H3 Cl	

CLASS INFORMATION

Class	Parent Substance

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CHEMFATE Search Results

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CAS #: 000075-01-4 Name: VINYL CHLORIDE

```
*******************************************************************************
MELT    VINYL CHLORIDE                                          CAS#    75-01-4
  Melting Point  :  -153.8      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      VINYL CHLORIDE                                          CAS#    75-01-4
  Vapor Pressure :  .2660E 04   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  VERSCHUEREN,K (1983)
*******************************************************************************

VP      VINYL CHLORIDE                                          CAS#    75-01-4
  Vapor Pressure :  2958        TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  EXTRAPULATED FROM MEASURED DATA USING ANTOINE EQUATION
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      VINYL CHLORIDE                                          CAS#    75-01-4
  Vapor Pressure :  .2320E 04   TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  PEARSON,CR & MCCONNELL,G (1975)
*******************************************************************************

VP      VINYL CHLORIDE                                          CAS#    75-01-4
  Vapor Pressure :  2981.6      MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

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End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Methylene chloride (dichloromethane)
CAS Number: 000075-09-2

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	6.0E-2	mg/kg/day	IRIS
Inhal RfD:	8.6E-1	mg/kg/day	HEAST
Oral Slope:	7.5E-3	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	1.6E-3	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	B2		
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	2.0E+3	mg/kg	ACGIH
Dermal LD50:		mg/kg	
Gas Inhal LC50:	1.2E+4	ppm	ACGIH
Dust Inhal LC50:	7.3E+4	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.4E+5	µg/L	ECOTOX
Salt Ecol LC50:	8.9E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	2.6E+5	days	CHEMFATE
Volatility:	8.1E+1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	2.6E+5	days	CHEMFATE
Volatility:	8.8E-1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
Log Kow:	1.3E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	8.5E+1	
Density:	1.3E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	4.3E+2	Torr	CHEMFATE
Henry's Law:	2.2E-3	atm-m3/mol	CHEMFATE
Water Solub:	1.3E+4	mg/L	CHEMFATE
Distrib Coef:	2.4E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	5.8E+2		ECOTOX
Salt BCF:			
Log Kow:	1.3E+0		CHEMFATE
Water Solub:	1.3E+4		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-9.5E+1	C
Boiling Point:	4.0E+1	C
Formula:	C H2 Cl2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-09-2 Name: METHYLENE DICHLORIDE

```
*******************************************************************************
MELT    METHYLENE DICHLORIDE                                    CAS#    75-09-2
  Melting Point  :  -94.92      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      METHYLENE DICHLORIDE                                    CAS#    75-09-2
  Vapor Pressure :  .2250E+03   .4090E+03   .7600E+03   TORR        MEASURED
  Temperature (C):  10.0        25.0        40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1966B)
*******************************************************************************

VP      METHYLENE DICHLORIDE                                    CAS#    75-09-2
  Vapor Pressure :  435         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      METHYLENE DICHLORIDE                                    CAS#    75-09-2
  Vapor Pressure :  433.14      MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

GALLANT,RW (1966B)
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RIDDICK,JA ET AL. (1986)

RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-25-2 Name: BROMOFORM

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*******************************************************************************
MELT    BROMOFORM                                          CAS#    75-25-2
  Melting Point  :  8.05        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      BROMOFORM                                          CAS#    75-25-2
  Vapor Pressure :  5.4         MM HG       CALC
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM DATA RANGE 30.000 TO 100.800 DEG C
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      BROMOFORM                                          CAS#    75-25-2
  Vapor Pressure :  5.51        MM HG       MEAS
  Temperature (C):  25
  Remarks        :  INTERPOLATED FROM DATA OBTAINED IN THE RANGE 8-423 DEG C,
                    SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Bromodichloromethane
CAS Number: 000075-27-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	2.0E-2	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:	6.2E-2	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	4.3E+2	mg/kg	RTECS
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	5.0E+4	days	CHEMFATE
Volatility:	1.1E+2	days	THOMAS
Photolysis:		days	
Biodeg:		days	
Radio:		days	
RIVER - Halflives			
Hydrolysis:	5.0E+4	days	CHEMFATE
Volatility:	1.2E+0	days	THOMAS
Photolysis:		days	
Biodeg:		days	
Radio:		days	
Log Kow:	2.1E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.6E+2	
Density:	2.0E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	5.0E+1	Torr	CHEMFATE
Henry's Law:	1.6E-3	atm-m3/mol	CHEMFATE
Water Solub:	6.7E+3	mg/L	CHEMFATE
Distrib Coef:	1.1E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.1E+0		CHEMFATE
Water Solub:	6.7E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-5.7E+1	C
Boiling Point:	9.0E+1	C
Formula:	C H Br Cl2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-27-4 Name: BROMODICHLOROMETHANE

```
*******************************************************************************
MELT    BROMODICHLOROMETHANE                                    CAS#    75-27-4
  Melting Point  :  -55          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*******************************************************************************

VP      BROMODICHLOROMETHANE                                    CAS#    75-27-4
  Vapor Pressure :  .50E 02      TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  US EPA (1981)
*******************************************************************************

VP      BROMODICHLOROMETHANE                                    CAS#    75-27-4
  Vapor Pressure :  50           MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************
```

ALDRICH (1988)
ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI: ALDRICH CHEM CO.; 1988

CALLAHAN,MA ET AL. (1979A)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS-VOLUME II.; EPA-440/4-79-029 WASHINGTON,DC: U.S. EPA.; 1979A

US EPA (1981)
U.S. EPA; TREATABILITY MANUAL I. TREATABILITY DATA.; EPA-600/2-82-001A. WASHINGTON,DC: U.S. EPA.; 1981

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-29-6
Chem Name  : 2-CHLOROPROPANE
Mol Formula: C3H7Cl
Mol Weight : 78.54
Melting Pt : -117.2 deg C
Boiling Pt : 35.7 deg C
Water Solubility:
   Value : 3100 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.90
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 515 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0175 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 9.2E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DONAGHY,T ET AL. (1993)
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dichloroethane, 1,1-

CAS Number: 000075-34-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	1.0E-1	mg/kg/day	LIVECHEM
Inhal RfD:	1.4E-1	mg/kg/day	HEAST
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:	1.3E+4	ppm	ACGIH
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	8.7E+1	days	THOMAS
Photolysis:		days	
Biodeg:	1.5E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	9.4E-1	days	THOMAS
Photolysis:		days	
Biodeg:	1.5E+2	days	FATERATE
Radio:		days	
Log Kow:	1.8E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	9.9E+1	
Density:	1.2E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.3E+2	Torr	CHEMFATE
Henry's Law:	5.6E-3	atm-m3/mol	CHEMFATE
Water Solub:	5.1E+3	mg/L	CHEMFATE
Distrib Coef:	6.3E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.8E+0		CHEMFATE
Water Solub:	5.1E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-9.7E+1	C
Boiling Point:	5.7E+1	C
Formula:	C2 H4 Cl2	

CLASS INFORMATION

Class	Parent Substance

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-34-3 Name: 1,1-DICHLOROETHANE

```
*******************************************************************************
MELT     1,1-DICHLOROETHANE                                    CAS#     75-34-3
  Melting Point  :  -96.96       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP       1,1-DICHLOROETHANE                                    CAS#     75-34-3
  Vapor Pressure :  227.3        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dichloroethylene, 1,1-
CAS Number: 000075-35-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	5.0E-2	mg/kg/day	IRIS
Inhal RfD:	5.7E-2	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:	1.2E+0	(mg/kg/day)^-1	HEAST
Inhal Wt-of-Evid:	C		
Oral ED10:	1.9E-1	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	C		
Inhal ED10:	1.9E-1	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	C		
Oral LD50:	1.9E+2	mg/kg	RTECS
Dermal LD50:	2.4E+3	mg/kg	RTECS
Gas Inhal LC50:	6.4E+3	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	9.0E+3	µg/L	ECOTOX
Salt Ecol LC50:	2.0E+5	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	8.7E+1	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	9.3E-1	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.1E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	9.7E+1	
Density:	1.2E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	6.0E+2	Torr	CHEMFATE
Henry's Law:	2.6E-2	atm-m3/mol	CHEMFATE
Water Solub:	2.3E+3	mg/L	CHEMFATE
Distrib Coef:	1.2E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.1E+0		CHEMFATE
Water Solub:	2.3E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.2E+2	C
Boiling Point:	3.2E+1	C
Formula:	C2 H2 Cl2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-35-4 Name: 1,1-DICHLOROETHYLENE

```
*******************************************************************************
MELT    1,1-DICHLOROETHYLENE                                    CAS#    75-35-4
  Melting Point  :  -122.56     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      1,1-DICHLOROETHYLENE                                    CAS#    75-35-4
  Vapor Pressure :  600         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1,1-DICHLOROETHYLENE                                    CAS#    75-35-4
  Vapor Pressure :  599.97      MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
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BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-43-4 Name: DICHLOROFLUOROMETHANE

```
*******************************************************************************
VP      DICHLOROFLUOROMETHANE                                   CAS#    75-43-4
  Vapor Pressure :  1.362E+03   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-43-4
Chem Name  : DICHLOROFLUOROMETHANE
Mol Formula: CHCl2F
Mol Weight : 102.92
Melting Pt : -135 deg C
Boiling Pt : 8.9 deg C
Water Solubility:
   Value : 1.88E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HORVATH,AL (1982)
Log P (octanol-water):
   Value : 1.55
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 1360 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0108 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.03E-014 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-45-6
Chem Name  : CHLORODIFLUOROMETHANE
Mol Formula: CHClF2
Mol Weight : 86.47
Melting Pt : -157.4 deg C
Boiling Pt : -40.7 deg C
Water Solubility:
   Value : 2770 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HORVATH,AL (1982)
Log P (octanol-water):
   Value : 1.08
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 7250 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : PERRY,RH & GREEN,D (1984)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0406 atm-m3/mole
   Temp  : 22 deg C
   Type  : EXP
   Ref   : CHANG,W & CRIDDLE,CS (1995)
Atmospheric OH Rate Constant:
   Value : 4.68E-015 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-61-6 Name: DIBROMODIFLUOROMETHANE

```
*******************************************************************************
VP      DIBROMODIFLUOROMETHANE                                  CAS#    75-61-6
  Vapor Pressure :  8.200E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-61-6
Chem Name  : DIBROMODIFLUOROMETHANE
Mol Formula: CBr2F2
Mol Weight : 209.82
Melting Pt : -110.1 deg C
Boiling Pt : 25 deg C
Water Solubility:
   Value : 313 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 1.99
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 820 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0308 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 5.9E-016 cm3/molecule-sec
   Temp  : 24 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1994);<5.9E-16
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-63-8
Chem Name  : BROMOTRIFLUOROMETHANE
Mol Formula: CBrF3
Mol Weight : 148.91
Melting Pt : -172 deg C
Boiling Pt : -57.8 deg C
Water Solubility:
   Value : 320 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HORVATH,AL (1982)
Log P (octanol-water):
   Value : 1.86
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 1.22E+004 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.499 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 1E-016 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1994);<1.0E-16
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trichlorofluoromethane
CAS Number: 000075-69-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	3.0E-1	mg/kg/day	IRIS
Inhal RfD:	2.0E-1	mg/kg/day	HEAST
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	3.7E+3	mg/kg	ACGIH
Dermal LD50:		mg/kg	
Gas Inhal LC50:	1.3E+5	ppm	ACGIH
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.0E+2	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.1E+0	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
Log Kow:	2.5E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.4E+2	
Density:	1.5E+0	g/mL @ 17.20 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	8.0E+2	Torr	CHEMFATE
Henry's Law:	9.7E-2	atm-m3/mol	CHEMFATE
Water Solub:	1.1E+3	mg/L	CHEMFATE
Distrib Coef:	2.4E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.5E+0		CHEMFATE
Water Solub:	1.1E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.1E+2	C
Boiling Point:	2.4E+1	C
Formula:	C Cl3 F	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-69-4 Name: TRICHLOROFLUOROMETHANE

```
*******************************************************************************
MELT    TRICHLOROFLUOROMETHANE                                  CAS#    75-69-4
  Melting Point  :  -110.48     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      TRICHLOROFLUOROMETHANE                                  CAS#    75-69-4
  Vapor Pressure :  .1455E 04   TORR        MEASURED
  Temperature (C):  21.
  Remarks        :  GAS
  Abbrev. Ref.   :  KAWAM,A & FLYNN,JB (1978)
*******************************************************************************

VP      TRICHLOROFLUOROMETHANE                                  CAS#    75-69-4
  Vapor Pressure :  802.8       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

KAWAM,A & FLYNN,JB (1978)
KAWAM,A.; FLYNN,J.B.; AEROSOLS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD. ED. 1:582-9.; 1978

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-71-8 Name: DICHLORODIFLUOROMETHANE

```
*******************************************************************************
MELT    DICHLORODIFLUOROMETHANE                                CAS#    75-71-8
  Melting Point  :  -158        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SMART,BE (1980)
*******************************************************************************

VP      DICHLORODIFLUOROMETHANE                                CAS#    75-71-8
  Vapor Pressure :  4847.8      MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

SMART,BE (1980)
SMART,B.E.; FLUORINATED ALIPHATIC COMPOUNDS.; IN: KIRK-OTHMER ENCYCL. CHEM TECH. 3RD ED. 10:856-70.; 1980

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-01-7 Name: PENTACHLOROETHANE

```
*******************************************************************************
MELT    PENTACHLOROETHANE                                        CAS#    76-01-7
  Melting Point  :  -29.0       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      PENTACHLOROETHANE                                        CAS#    76-01-7
  Vapor Pressure :  3.5         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ENGINEERING SCIENCES DATA UNIT (1976)
*******************************************************************************
```

ENGINEERING SCIENCES DATA UNIT (1976)
ENGINEERING SCIENCES DATA UNIT.; VAPOR PRESSURES AND CRITICAL POINTS OF LIQUIDS. VII. HALOGENATED ETHANES AND ETHYLENES.; ENG. SCI. DATA ITEM. 76004. PP.43.; 1976

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-03-9 Name: TRICHLOROACETIC ACID

```
*******************************************************************************
VP      TRICHLOROACETIC ACID                                    CAS#    76-03-9
  Vapor Pressure :  .1E 01      TORR        MEASURED
  Temperature (C):  51.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*******************************************************************************
```

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000076-03-9
Chem Name  : TRICHLOROACETIC ACID
Mol Formula: C2HCl3O2
Mol Weight : 163.39
Melting Pt : 57.5 deg C
Boiling Pt : 196.5 deg C
Water Solubility:
   Value : 4.4E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.33
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.06 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : PERRY,RH & GREEN, D (1984)
pKa Dissociation Constant:
   Value : 0.51
   Temp  :
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 1.35E-008 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BOWDEN,DJ ET AL. (1998)
Atmospheric OH Rate Constant:
   Value : 5.2E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000076-11-9
Chem Name  : 1,1,1,2-TETRACHLORO-2,2-DIFLUOROETHANE
Mol Formula: C2Cl4F2
Mol Weight : 203.83
Melting Pt : 40.6 deg C
Boiling Pt : 91.5 deg C
Water Solubility:
   Value : 100 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ROY,WR & GRIFFIN,RA (1985)
Log P (octanol-water):
   Value : 3.41
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 60 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1998)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.161 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-12-0 Name: 1,1,2,2,-TETRACHLORODIFLUOROETHANE

```
*******************************************************************************
VP      1,1,2,2,-TETRACHLORODIFLUOROETHANE                    CAS#    76-12-0
  Vapor Pressure :  2.202E+04   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000076-12-0
Chem Name  : 1,1,2,2,-TETRACHLORODIFLUOROETHANE
Mol Formula: C2Cl4F2
Mol Weight : 203.83
Melting Pt : 26 deg C
Boiling Pt : 93 deg C
Water Solubility:
   Value : 120 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 3.41
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 50.5 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.113 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-13-1 Name: 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE

```
*******************************************************************************
MELT    1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE              CAS#    76-13-1
  Melting Point  :  -36.4       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE              CAS#    76-13-1
  Vapor Pressure :  362.5       MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE              CAS#    76-13-1
  Vapor Pressure :  331.622     MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-14-2 Name: 1,2-DICHLORO-1,1,2,2-TETRAFLUOROETHANE

```
*******************************************************************************
MELT    1,2-DICHLORO-1,1,2,2-TETRAFLUOROETHANE            CAS#    76-14-2
  Melting Point  :  -94         DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      1,2-DICHLORO-1,1,2,2-TETRAFLUOROETHANE            CAS#    76-14-2
  Vapor Pressure :  2014        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000076-15-3 Name: CHLOROPENTAFLUOROETHANE

```
*****************************************************************************
VP      CHLOROPENTAFLUOROETHANE                          CAS#     76-15-3
  Vapor Pressure :  .7598E 03   TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  SMART,BE (1980)
*****************************************************************************
```

SMART,BE (1980)
SMART,B.E.; FLUORINATED ALIPHATIC COMPOUNDS.; IN: KIRK-OTHMER ENCYCL. CHEM TECH. 3RD ED. 10:856-70.; 1980

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000076-15-3
Chem Name  : CHLOROPENTAFLUOROETHANE
Mol Formula: C2ClF5
Mol Weight : 154.47
Melting Pt : -99.4 deg C
Boiling Pt : -37.9 deg C
Water Solubility:
   Value : 58 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HORVATH,AL (1982)
Log P (octanol-water):
   Value : 2.47
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 6860 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 5.58 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000764-41-0
Chem Name  : 1,4-DICHLORO-2-BUTENE
Mol Formula: C4H6Cl2
Mol Weight : 125.00
Melting Pt : 3.5 deg C
Boiling Pt : 158 deg C
Water Solubility:
   Value : 580 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ALBANESE,V ET AL. (1987)
Log P (octanol-water):
   Value : 2.60
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 3 mm Hg
   Temp  :
   Type  : EXP
   Ref   : ALBANESE,V ET AL. (1987)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.00851 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.33E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dichloropropane, 1,2-
CAS Number: 000078-87-5

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:	1.1E-3	mg/kg/day	IRIS
Oral Slope:	6.8E-2	(mg/kg/day)^-1	HEAST
Oral Wt-of-Evid:	B2		
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	2.0E+3	mg/kg	ACGIH
Dermal LD50:	8.8E+3	mg/kg	RTECS
Gas Inhal LC50:	7.2E+2	ppm	ACGIH
Dust Inhal LC50:	1.2E+4	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	4.2E+4	µg/L	ECOTOX
Salt Ecol LC50:	5.3E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	6.7E+6	days	CHEMFATE
Volatility:	9.3E+1	days	THOMAS
Photolysis:		days	
Biodeg:	1.3E+3	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	6.7E+6	days	CHEMFATE
Volatility:	1.0E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.3E+3	days	FATERATE
Radio:		days	
Log Kow:	2.0E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.1E+2	
Density:	1.2E+0	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	5.2E+1	Torr	CHEMFATE
Henry's Law:	2.8E-3	atm-m3/mol	CHEMFATE
Water Solub:	2.8E+3	mg/L	CHEMFATE
Distrib Coef:	8.7E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.0E+0		CHEMFATE
Water Solub:	2.8E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-7.0E+1	C
Boiling Point:	9.6E+1	C
Formula:	C3 H6 Cl2	

CLASS INFORMATION

Class	Parent Substance

Syracuse Research Corporation
Search Contact Us
About SRC Locations Business Areas Career Center Training

CHEMFATE Search Results

Return to EFDB page

CAS #: 000078-87-5 Name: 1,2-DICHLOROPROPANE

```
*******************************************************************************
MELT    1,2-DICHLOROPROPANE                                    CAS#    78-87-5
  Melting Point  :  -100        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*******************************************************************************

VP      1,2-DICHLOROPROPANE                                    CAS#    78-87-5
  Vapor Pressure :  .42E 02     TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  US EPA (1981)
*******************************************************************************

VP      1,2-DICHLOROPROPANE                                    CAS#    78-87-5
  Vapor Pressure :  .3000E+02   .5200E+02   .1030E+03   TORR        MEASURED
  Temperature (C):  10.0        25.0        40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1966A)
*******************************************************************************

VP      1,2-DICHLOROPROPANE                                    CAS#    78-87-5
  Vapor Pressure :  53.3        MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1,2-DICHLOROPROPANE                                    CAS#    78-87-5
  Vapor Pressure :  51.989      MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

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GALLANT,RW (1966A)
GALLANT,R.W.; PHYSICAL PROPERTIES OF HYDROCARBONS. VII.CHLORINATED ALIPHATICS.; HYDROCARBON PROCESS.; 45:111-18.; 1966A

US EPA (1981)
U.S. EPA; TREATABILITY MANUAL I. TREATABILITY DATA.; EPA-600/2-82-001A. WASHINGTON,DC: U.S. EPA.; 1981

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trichloroethane, 1,1,2-
CAS Number: 000079-00-5

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	4.0E-3	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:	5.7E-2	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	C		
Inhal Slope:	5.7E-2	(mg/kg/day)^-1	HEAST
Inhal Wt-of-Evid:	C		
Oral ED10:	2.8E+0	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	C		
Inhal ED10:	2.8E+0	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	C		
Oral LD50:	3.8E+2	mg/kg	ACGIH
Dermal LD50:	5.4E+3	mg/kg	RTECS
Gas Inhal LC50:	5.0E+2	ppm	RTECS
Dust Inhal LC50:	1.3E+1	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	4.2E+3	µg/L	ECOTOX
Salt Ecol LC50:	3.4E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.4E+4	days	FATERATE
Volatility:	1.0E+2	days	THOMAS
Photolysis:		days	
Biodeg:	3.7E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.4E+4	days	FATERATE
Volatility:	1.1E+0	days	THOMAS
Photolysis:		days	
Biodeg:	3.7E+2	days	FATERATE
Radio:		days	
Log Kow:	2.0E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.3E+2	
Density:	1.4E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.3E+1	Torr	CHEMFATE
Henry's Law:	9.1E-4	atm-m3/mol	CHEMFATE
Water Solub:	4.4E+3	mg/L	CHEMFATE
Distrib Coef:	1.0E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.0E+0		CHEMFATE
Water Solub:	4.4E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-3.7E+1	C
Boiling Point:	1.1E+2	C
Formula:	C2 H3 Cl3	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-00-5 Name: 1,1,2-TRICHLOROETHANE

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*******************************************************************************
MELT    1,1,2-TRICHLOROETHANE                                   CAS#    79-00-5
  Melting Point  :  -35          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      1,1,2-TRICHLOROETHANE                                   CAS#    79-00-5
  Vapor Pressure :  23           MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  ENGINEERING SCIENCES DATA UNIT (1976)
*******************************************************************************

VP      1,1,2-TRICHLOROETHANE                                   CAS#    79-00-5
  Vapor Pressure :  23.25        MM HG        MEASE
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

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MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trichloroethylene (TCE)
CAS Number: 000079-01-6

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:		mg/kg/day	
Oral Slope:	1.1E-2	(mg/kg/day)^-1	LIVECHEM
Oral Wt-of-Evid:	B2		
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:	1.0E+1	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	1.0E+1	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	6.0E+3	mg/kg	ACGIH
Dermal LD50:	2.0E+4	mg/kg	RTECS
Gas Inhal LC50:	4.8E+3	ppm	RTECS
Dust Inhal LC50:	3.3E+1	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.9E+3	µg/L	ECOTOX
Salt Ecol LC50:	1.2E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.2E+2	days	FATERATE
Volatility:	1.0E+2	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.2E+2	days	FATERATE
Volatility:	1.1E+0	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
Log Kow:	2.4E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.3E+2	
Density:	1.5E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	7.3E+1	Torr	CHEMFATE
Henry's Law:	1.0E-2	atm-m3/mol	CHEMFATE
Water Solub:	1.5E+3	mg/L	CHEMFATE
Distrib Coef:	3.3E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	1.7E+1		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	1.7E+1		ECOTOX
Salt BCF:			
Log Kow:	2.4E+0		CHEMFATE
Water Solub:	1.5E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-8.5E+1	C
Boiling Point:	8.7E+1	C
Formula:	C2 H Cl3	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-01-6 Name: TRICHLOROETHYLENE

```
*******************************************************************************
MELT    TRICHLOROETHYLENE                                    CAS#    79-01-6
  Melting Point  :  -84.8       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      TRICHLOROETHYLENE                                    CAS#    79-01-6
  Vapor Pressure :  .58E 02     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  FROM JOHN,R. (1976)
  Abbrev. Ref.   :  ROGERS,RD & MCFARLANE,JC (1981)
*******************************************************************************

VP      TRICHLOROETHYLENE                                    CAS#    79-01-6
  Vapor Pressure :  69          MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      TRICHLOROETHYLENE                                    CAS#    79-01-6
  Vapor Pressure :  73.46       MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
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ROGERS,RD & MCFARLANE,JC (1981)

ROGERS,R.D.; MCFARLANE,J.C.; SORPTION OF CARBON TETRACHLORIDE, ETHYLENE DIBROMIDE AND TRICHLOROETHYLENE IN SOIL AND CLAY.; ENVIRON. MONIT. ASSESS.; 1:155-8.; 1981

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Tetrachloroethane, 1,1,2,2-
CAS Number: 000079-34-5

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:		mg/kg/day	
Oral Slope:	2.0E-1	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	C		
Inhal Slope:	2.0E-1	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	C		
Oral ED10:	6.0E-1	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	C		
Inhal ED10:	6.0E-1	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	C		
Oral LD50:	3.2E+2	mg/kg	ACGIH
Dermal LD50:	6.3E+3	mg/kg	ACGIH
Gas Inhal LC50:	1.0E+3	ppm	ACGIH
Dust Inhal LC50:	3.7E+3	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	4.4E+1	days	FATERATE
Volatility:	1.1E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	4.4E+1	days	FATERATE
Volatility:	1.3E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.4E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.7E+2	
Density:	1.6E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	4.6E+0	Torr	CHEMFATE
Henry's Law:	3.4E-4	atm-m3/mol	CHEMFATE
Water Solub:	3.0E+3	mg/L	CHEMFATE
Distrib Coef:	1.9E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	8.0E+0		VER_BCF
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	8.0E+0		VER_BCF
Salt BCF:			
Log Kow:	2.4E+0		CHEMFATE
Water Solub:	3.0E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-4.4E+1	C
Boiling Point:	1.5E+2	C
Formula:	C2 H2 Cl4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-34-5 Name: 1,1,2,2-TETRACHLOROETHANE

```
*******************************************************************************
MELT    1,1,2,2-TETRACHLOROETHANE                          CAS#    79-34-5
  Melting Point  :  -44          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      1,1,2,2-TETRACHLOROETHANE                          CAS#    79-34-5
  Vapor Pressure :  6.1          MM HG       MEAS
  Temperature (C):  25
  Abbrev. Ref.   :  ENGINEERING SCIENCES DATA UNIT (1976)
*******************************************************************************

VP      1,1,2,2-TETRACHLOROETHANE                          CAS#    79-34-5
  Vapor Pressure :  4.620E+00    MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************

VP      1,1,2,2-TETRACHLOROETHANE                          CAS#    79-34-5
  Vapor Pressure :  4.62         MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

ENGINEERING SCIENCES DATA UNIT (1976)
ENGINEERING SCIENCES DATA UNIT.; VAPOR PRESSURES AND CRITICAL POINTS OF LIQUIDS. VII. HALOGENATED ETHANES AND ETHYLENES.; ENG. SCI. DATA ITEM. 76004. PP.43.; 1976

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH

ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dibromo-3-chloropropane, 1,2-
CAS Number: 000096-12-8

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:	5.7E-5	mg/kg/day	IRIS
Oral Slope:	1.4E+0	(mg/kg/day)^-1	HEAST
Oral Wt-of-Evid:	B2		
Inhal Slope:	2.4E-3	(mg/kg/day)^-1	HEAST
Inhal Wt-of-Evid:	B2		
Oral ED10:	8.1E-4	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	8.1E-4	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	1.5E+2	mg/kg	RTECS
Dermal LD50:	1.4E+3	mg/kg	RTECS
Gas Inhal LC50:	1.0E+2	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.0E+4	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.4E+2	days	CHEMFATE
Volatility:	1.4E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.4E+2	days	CHEMFATE
Volatility:	1.7E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.3E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.4E+2	
Density:	2.1E+0	g/mL @ 14.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	5.8E-1	Torr	CHEMFATE
Henry's Law:	1.5E-4	atm-m3/mol	CHEMFATE
Water Solub:	1.2E+3	mg/L	CHEMFATE
Distrib Coef:	1.7E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.3E+0		CHEMFATE
Water Solub:	1.2E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:		C
Boiling Point:	2.0E+2	C
Formula:	C3 H5 Br2 Cl	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000096-12-8 Name: 1,2-DIBROMO-3-CHLOROPROPANE

```
*******************************************************************************
MELT    1,2-DIBROMO-3-CHLOROPROPANE                          CAS#    96-12-8
  Melting Point  :  6            DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  STENGER,VA (1978)
*******************************************************************************

VP      1,2-DIBROMO-3-CHLOROPROPANE                          CAS#    96-12-8
  Vapor Pressure :  0.58         MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MUNNECKE,DE & VANGUNDY,SD (1979)
*******************************************************************************
```

MUNNECKE,DE & VANGUNDY,SD (1979)
MUNNECKE,D.E.; VANGUNDY,S.D.; MOVEMENT OF FUMIGANTS IN SOIL, DOSAGE, RESPONSES, AND DIFFERENTIAL EFFECTS.; ANNU. REV. PHYTOPATHOL.; 17:405-29; 1979

STENGER,VA (1978)
STENGER,V.A.; BROMINE COMPOUNDS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECHNOL. 3 ED. NEW YORK,NY: WILEY-INTERSCIENCE. 4:243-63; 1978

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trichloropropane, 1,2,3-
CAS Number: 000096-18-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	6.0E-3	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:	7.0E+0	(mg/kg/day)^-1	HEAST
Oral Wt-of-Evid:	B2		
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	3.4E+2	mg/kg	ACGIH
Dermal LD50:	5.2E+2	mg/kg	RTECS
Gas Inhal LC50:	5.0E+2	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.6E+4	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.6E+4	days	CHEMFATE
Volatility:	1.1E+2	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.6E+4	days	CHEMFATE
Volatility:	1.2E+0	days	THOMAS
Photolysis:		days	
Biodeg:	3.6E+2	days	FATERATE
Radio:		days	
Log Kow:	2.0E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.5E+2	
Density:	1.4E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	3.7E+0	Torr	CHEMFATE
Henry's Law:	4.1E-4	atm-m3/mol	CHEMFATE
Water Solub:	1.8E+3	mg/L	CHEMFATE
Distrib Coef:	1.4E-1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.0E+0		CHEMFATE
Water Solub:	1.8E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.5E+1	C
Boiling Point:	1.6E+2	C
Formula:	C3 H5 Cl3	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000096-18-4 Name: 1,2,3-TRICHLOROPROPANE

```
*******************************************************************************
MELT     1,2,3-TRICHLOROPROPANE                                CAS#     96-18-4
  Melting Point  :  -14.7        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP       1,2,3-TRICHLOROPROPANE                                CAS#     96-18-4
  Vapor Pressure :  3.1          MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  MACKAY,D ET AL. (1982)
*******************************************************************************

VP       1,2,3-TRICHLOROPROPANE                                CAS#     96-18-4
  Vapor Pressure :  3.687E+00    MM HG        MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

MACKAY,D ET AL. (1982)
MACKAY,D.; BOBRA,A.; CHAN,D.W.; SHIU,W.Y.; VAPOR PRESSURE CORRELATIONS FOR LOW-VOLATILITY ENVIRONMENTAL CHEMICALS.; ENVIRON. SCI. TECHNOL.; 16:645-9.; 1982

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

WTP RISK ASSESSMENT WORK PLAN IDENTIFIED CONSTITUENTS OF POTENTIAL CONCERN (COPC) SUPPORT DATA

Non-aromatic Nonhalogenated Hydrocarbons (NANHH)

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000106-35-4
Chem Name  : 3-HEPTANONE
Mol Formula: C7H14O
Mol Weight : 114.19
Melting Pt : -39 deg C
Boiling Pt : 147 deg C
Water Solubility:
   Value : 4300 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : FLICK,EW (1991)
Log P (octanol-water):
   Value : 1.73
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 2.6 mm Hg
   Temp  : 20 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1993)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.08E-005 atm-m3/mole
   Temp  : 20 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 7.89E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-88-7 Name: 1-BUTENE OXIDE

```
*******************************************************************************
MELT    1-BUTENE OXIDE                                          CAS#   106-88-7
  Melting Point  :  -150        DEGC
  Remarks        :  SETS TO A GLASS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HAWLEY,GG (1981)
*******************************************************************************

VP      1-BUTENE OXIDE                                          CAS#   106-88-7
  Vapor Pressure :  .176E 03    TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  BOGYO,DA ET AL. (1980)
*******************************************************************************

VP      1-BUTENE OXIDE                                          CAS#   106-88-7
  Vapor Pressure :  180         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  OSBORN,AG & SCOTT,DW (1980)
*******************************************************************************
```

BOGYO,DA ET AL. (1980)
BOGYO,D.A.; LANDE,S.S.; MEYLEN,W.M.; HOWARD,P.H.; SANTODONATO,J.;
INVESTIGATION OF SELECTED ENVIRONMENTAL CONTAMINANTS: EPOXIDES.;
EPA-560/11-80-005. WASHINGTON,D.C.:US EPA. PP.202.; 1980

HAWLEY,GG (1981)
HAWLEY,G.G.; THE CONDENSED CHEMICAL DISTIONARY. 10TH ED.; NEW YORK,NY: VAN
NOSTRAND REINHOLD CO. PP.1135.; 1981

OSBORN,AG & SCOTT,DW (1980)
OSBORN,A.G.; SCOTT,D.W.; VAPOR PRESSURE OF 17 MISCELLANEOUS ORGANIC COMPOUN
J CHEM THERMODYNAMIC; 12:429-38; 1980

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-97-8 Name: BUTANE

```
*****************************************************************************
MELT    BUTANE                                                  CAS#   106-97-8
  Melting Point  :  -138.4      DEG C
  Remarks        :
              1  :  LIDE (1991)
              2  :   HPV: LOW 1,3-BUTADIENE C4 STREAMS
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************

VP      BUTANE                                                  CAS#   106-97-8
  Vapor Pressure :  2800        MM HG       MEASURED
  Temperature (C):  40
  Remarks        :
              1  :  GAS PRODUCERS ASSOCIATION (1996)
              2  :   HPV: LOW 1,3-BUTADIENE C4 STREAMS
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************
```

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000106-97-8
Chem Name  : N-BUTANE
Mol Formula: C4H10
Mol Weight : 58.12
Melting Pt : -138.2 deg C
Boiling Pt : -0.5 deg C
Water Solubility:
   Value : 61.2 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : MCAULIFFE,C (1966)
Log P (octanol-water):
   Value : 2.89
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 1820 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.95 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 2.54E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-99-0 Name: 1,3-BUTADIENE

```
*******************************************************************************
MELT     1,3-BUTADIENE                                          CAS#   106-99-0
  Melting Point  :  -108.966     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP       1,3-BUTADIENE                                          CAS#   106-99-0
  Vapor Pressure :  2107         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Acrolein

CAS Number: 000107-02-8

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	5.0E-4	mg/kg/day	IRIS
Inhal RfD:	5.7E-6	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	4.6E+1	mg/kg	ACGIH
Dermal LD50:	5.6E+2	mg/kg	ACGIH
Gas Inhal LC50:	6.6E+1	ppm	RTECS
Dust Inhal LC50:	1.5E+1	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	6.0E+0	µg/L	ECOTOX
Salt Ecol LC50:	2.7E+2	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	5.0E-1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	5.0E-1	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
Log Kow:	-1.0E-2		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	5.6E+1	
Density:	8.4E-1	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.7E+2	Torr	CHEMFATE
Henry's Law:	1.2E-4	atm-m3/mol	CHEMFATE
Water Solub:	2.1E+5	mg/L	CHEMFATE
Distrib Coef:	1.5E-1	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	3.4E+2		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	3.4E+2		ECOTOX
Salt BCF:			
Log Kow:	-1.0E-2		CHEMFATE
Water Solub:	2.1E+5		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-8.8E+1	C
Boiling Point:	5.3E+1	C
Formula:	C3 H4 O	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-02-8 Name: ACROLEIN

```
*******************************************************************************
MELT    ACROLEIN                                              CAS#   107-02-8
  Melting Point  :  -86.95      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      ACROLEIN                                              CAS#   107-02-8
  Vapor Pressure :  .220E 03    TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  HESS,LG ET AL. (1978)
*******************************************************************************

VP      ACROLEIN                                              CAS#   107-02-8
  Vapor Pressure :  273         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  STULL,DR (1947)
*******************************************************************************

VP      ACROLEIN                                              CAS#   107-02-8
  Vapor Pressure :  2.741E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

HESS,LG ET AL. (1978)
HESS,L.G.; KURTZ,A.N.; STANTON,D.B.; ACROLEIN AND DERIVATIVES.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 1:277-97.; 1978

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

STULL,DR (1947)
STULL,D.R.; VAPOR PRESSURE OF PURE SUBSTANCES-ORGANIC COMPOUNDS.; IND. ENG. CHEM.; 39:517-50.; 1947

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-12-0 Name: PROPIONITRILE

```
*******************************************************************************
MELT    PROPIONITRILE                                          CAS#   107-12-0
  Melting Point  :  -91.8        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      PROPIONITRILE                                          CAS#   107-12-0
  Vapor Pressure :  40           MM HG
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      PROPIONITRILE                                          CAS#   107-12-0
  Vapor Pressure :  4.739E+01    MM HG        MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-13-1 Name: ACRYLONITRILE

```
*******************************************************************************
MELT    ACRYLONITRILE                                          CAS#   107-13-1
  Melting Point  :  -83.55      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      ACRYLONITRILE                                          CAS#   107-13-1
  Vapor Pressure :  .5000E+02   .1000E+03   .1100E+03   TORR        MEASURED
  Temperature (C):  8.7         23.6        25.0
  Abbrev. Ref.   :  NORRIS,MV (1967)
*******************************************************************************

VP      ACRYLONITRILE                                          CAS#   107-13-1
  Vapor Pressure :  108.5       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

NORRIS,MV (1967)
NORRIS,M.V.; ACRYLONITRILE.; ENCYCL. IND. CHEM. ANAL.; 4:368-81.; 1967

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-18-6 Name: ALLYL ALCOHOL

```
*******************************************************************************
MELT    ALLYL ALCOHOL                                          CAS#   107-18-6
  Melting Point  :  -129        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*******************************************************************************

VP      ALLYL ALCOHOL                                          CAS#   107-18-6
  Vapor Pressure :  28.1        MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      ALLYL ALCOHOL                                          CAS#   107-18-6
  Vapor Pressure :  2.610E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

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ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI: ALDRICH CHEM CO.; 1988

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-19-7 Name: PROPARGYLIC ALCOHOL

```
*******************************************************************************
MELT     PROPARGYLIC ALCOHOL                                    CAS#   107-19-7
  Melting Point  :  -51.8        DEG C
  Remarks        :
             1   :  CRC HNDBK CHEM PHYS 81ST ED. (2000)
             2   :   HPV: PROPARGYL ALCOHOL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************

VP       PROPARGYLIC ALCOHOL                                    CAS#   107-19-7
  Vapor Pressure :  1.560E+01    MM HG        MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************

VP       PROPARGYLIC ALCOHOL                                    CAS#   107-19-7
  Vapor Pressure :  15.6         MM HG        CALCULATED
  Temperature (C):  25
  Remarks        :
             1   :  DAUBERT AND DANNER (1989)
             2   :   HPV: PROPARGYL ALCOHOL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-31-3 Name: METHYL FORMATE

```
*******************************************************************************
VP      METHYL FORMATE                                          CAS#   107-31-3
  Vapor Pressure :  5.857E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000107-31-3
Chem Name  : METHYLFORMATE
Mol Formula: C2H4O2
Mol Weight : 60.05
Melting Pt : -99 deg C
Boiling Pt : 31.7 deg C
Water Solubility:
   Value : 2.3E+005 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 0.03
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 586 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000223 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 2.27E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-87-9 Name: METHYL PROPYL KETONE

```
*******************************************************************************
MELT    METHYL PROPYL KETONE                                    CAS#   107-87-9
  Melting Point  :  -78          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

MELT    METHYL PROPYL KETONE                                    CAS#   107-87-9
  Melting Point  :  -78          DEG C
  Remarks        :
             1   :  MERCK INDEX (1996)
             2   :   HPV: METHYL N-PROPYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************

VP      METHYL PROPYL KETONE                                    CAS#   107-87-9
  Vapor Pressure :  35.4         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      METHYL PROPYL KETONE                                    CAS#   107-87-9
  Vapor Pressure :  35.4         MM HG        MEASURED
  Temperature (C):  25
  Remarks        :
             1   :  RIDDICK ET AL. (1985)
             2   :   HPV: METHYL N-PROPYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE

HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-98-2 Name: 1-METHOXY-2-PROPANOL

```
*******************************************************************************
MELT    1-METHOXY-2-PROPANOL                                  CAS#   107-98-2
  Melting Point  :  -142        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*******************************************************************************

VP      1-METHOXY-2-PROPANOL                                  CAS#   107-98-2
  Vapor Pressure :  12.5        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*******************************************************************************
```

DOW CHEMICAL COMPANY (1981)
DOW CHEMICAL COMPANY.; THE GLYCOL ETHERS HANDBOOK.; MIDLAND, MI: DOW CHEMICAL CO.; 1981

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000108-03-2
Chem Name  : 1-NITROPROPANE
Mol Formula: C3H7NO2
Mol Weight : 89.10
Melting Pt : -108 deg C
Boiling Pt : 131.1 deg C
Water Solubility:
   Value : 1.5E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 0.87
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 10.1 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 8.98
   Temp  :
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Henry's Law Constant:
   Value : 8.7E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 4.4E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Vinyl acetate
CAS Number: 000108-05-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	1.0E+0	mg/kg/day	HEAST
Inhal RfD:	5.7E-2	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	1.6E+3	mg/kg	ACGIH
Dermal LD50:	2.3E+3	mg/kg	ACGIH
Gas Inhal LC50:	2.5E+3	ppm	ACGIH
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.4E+4	µg/L	ECOTOX
Salt Ecol LC50:	1.0E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	7.3E+0	days	CHEMFATE
Volatility:	8.2E+1	days	THOMAS
Photolysis:	2.7E-1	days	CHEMFATE
Biodeg:		days	
Radio:		days	
RIVER - Halflives			
Hydrolysis:	7.3E+0	days	CHEMFATE
Volatility:	9.2E-1	days	THOMAS
Photolysis:	2.7E-1	days	CHEMFATE
Biodeg:		days	
Radio:		days	
Log Kow:	7.3E-1		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	8.6E+1	
Density:	9.3E-1	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	9.0E+1	Torr	CHEMFATE
Henry's Law:	5.1E-4	atm-m3/mol	CHEMFATE
Water Solub:	2.0E+4	mg/L	CHEMFATE
Distrib Coef:	7.9E-1	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	7.3E-1		CHEMFATE
Water Solub:	2.0E+4		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-9.3E+1	C
Boiling Point:	7.3E+1	C
Formula:	C4 H6 O2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-05-4 Name: VINYL ACETATE

```
*******************************************************************************
MELT    VINYL ACETATE                                          CAS#   108-05-4
  Melting Point  :  -92.8        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      VINYL ACETATE                                          CAS#   108-05-4
  Vapor Pressure :  90.16        MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Methyl isobutyl ketone
CAS Number: 000108-10-1

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	8.0E-2	mg/kg/day	HEAST
Inhal RfD:	8.6E-1	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	2.1E+3	mg/kg	ACGIH
Dermal LD50:	3.0E+3	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:	8.3E+4	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	4.6E+5	µg/L	ECOTOX
Salt Ecol LC50:	1.2E+6	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	8.8E+1	days	THOMAS
Photolysis:		days	
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.1E+0	days	THOMAS
Photolysis:		days	
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
Log Kow:	1.2E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.0E+2	
Density:	8.0E-1	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.0E+1	Torr	CHEMFATE
Henry's Law:	1.4E-4	atm-m3/mol	CHEMFATE
Water Solub:	1.9E+4	mg/L	CHEMFATE
Distrib Coef:	2.2E+0	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.2E+0		CHEMFATE
Water Solub:	1.9E+4		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-8.4E+1	C
Boiling Point:	1.2E+2	C
Formula:	C6 H12 O	

CLASS INFORMATION

Class	Parent Substance

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-10-1 Name: METHYL ISOBUTYL KETONE

```
*******************************************************************************
MELT    METHYL ISOBUTYL KETONE                                  CAS#   108-10-1
  Melting Point  :  -84          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      METHYL ISOBUTYL KETONE                                  CAS#   108-10-1
  Vapor Pressure :  .188E 02     TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1975)
*******************************************************************************

VP      METHYL ISOBUTYL KETONE                                  CAS#   108-10-1
  Vapor Pressure :  .16E 02      TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  HANN,RWJR & JENSEN,PA (1977)
*******************************************************************************

VP      METHYL ISOBUTYL KETONE                                  CAS#   108-10-1
  Vapor Pressure :  19.86        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

AMBROSE,D ET AL. (1975)
AMBROSE,D.; ELLENDER,J.H.; LEES,E.B.; SPRAKE,C.H.S.; TOWNSEND,R.; THERMODYNAMIC PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. XXXVIII. VAPOUR PRESSURES OF SOME ALIPHATIC KETONES.; J. CHEM. THERM.; 7:453-72.; 1975

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

HANN,RWJR & JENSEN,PA (1977)
HANN,R.W. JR.; JENSEN,P.A.; WATER QUALITY CHARACTERISTICS OF HAZARDOUS MATERIALS.; NTIS-PB-285946. TEXAS A&M UNIV., COLLEGE STATION ENVIRONMENTAL ENGINEERING DIV. 1751 PP.; 1977

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-20-3 Name: DIISOPROPYL ETHER

```
*******************************************************************************
VP      DIISOPROPYL ETHER                                   CAS#   108-20-3
  Vapor Pressure :  .130E 03    TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*******************************************************************************

VP      DIISOPROPYL ETHER                                   CAS#   108-20-3
  Vapor Pressure :  .1491E 03   TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1976)
*******************************************************************************
```

AMBROSE,D ET AL. (1976)
AMBROSE,D.; ELLENDER,J.H.; SPRAKE, C.H.S.; TOWNSEND, R.; THERMODYNAMIC PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. XLIII. VAPOR PRESSURES OF SOME ETHERS.; J. CHEM. THERMODYN.; 8:165-78.; 1976

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000108-20-3
Chem Name  : DI-ISOPROPYL ETHER
Mol Formula: C6H14O
Mol Weight : 102.18
Melting Pt : -86.8 deg C
Boiling Pt : 68.5 deg C
Water Solubility:
   Value : 8800 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : HEITMANN,W ET AL (1987)
Log P (octanol-water):
   Value : 1.52
   Type  : EXP
   Ref   : FUNASAKI,N ET AL. (1985)
Vapor Pressure:
   Value : 149 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1995)
pKa Dissociation Constant:
   Value : -4.3
   Temp  :
   Type  : EXP
   Ref   : PERRIN,DD (1965)
Henry's Law Constant:
   Value : 0.00228 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.02E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000108-87-2
Chem Name  : 1-METHYLCYCLOHEXANE
Mol Formula: C7H14
Mol Weight : 98.19
Melting Pt : -126.6 deg C
Boiling Pt : 100.9 deg C
Water Solubility:
   Value : 14 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 3.61
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 46 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.43 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 1.04E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-94-1 Name: CYCLOHEXANONE

```
*******************************************************************************
VP      CYCLOHEXANONE                                          CAS#   108-94-1
  Vapor Pressure :  .45E 01     TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  HANN,RWJR & JENSEN,PA (1977)
*******************************************************************************

VP      CYCLOHEXANONE                                          CAS#   108-94-1
  Vapor Pressure :  4.330E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

HANN,RWJR & JENSEN,PA (1977)
HANN,R.W. JR.; JENSEN,P.A.; WATER QUALITY CHARACTERISTICS OF HAZARDOUS MATERIALS.; NTIS-PB-285946. TEXAS A&M UNIV., COLLEGE STATION ENVIRONMENTAL ENGINEERING DIV. 1751 PP.; 1977

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000108-94-1
Chem Name  : CYCLOHEXANONE
Mol Formula: C6H10O
Mol Weight : 98.15
Melting Pt : -31 deg C
Boiling Pt : 155.4 deg C
Water Solubility:
   Value : 2.5E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.81
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 4.33 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value : 11.3
   Temp  :
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 9E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HAWTHORNE,SB ET AL. (1985)
Atmospheric OH Rate Constant:
   Value : 6.39E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

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CAS #: 000109-66-0 Name: N-PENTANE

```
*****************************************************************************
MELT    N-PENTANE                                          CAS#   109-66-0
  Melting Point  :  -130        DEG C
  Remarks        :
             1   :  LIDE (1991)
             2   :   HPV: PETROLEUM GAS
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************

VP      N-PENTANE                                          CAS#   109-66-0
  Vapor Pressure :  860         MM HG       MEASURED
  Temperature (C):  40
  Remarks        :
             1   :  GAS PRODUCERS ASSOCIATION (1996)
             2   :   HPV: PETROLEUM GAS
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************
```

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

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```
CAS Number : 000109-66-0
Chem Name  : N-PENTANE
Mol Formula: C5H12
Mol Weight : 72.15
Melting Pt : -129.7 deg C
Boiling Pt : 36 deg C
Water Solubility:
   Value : 38 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 3.39
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 514 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 1.25 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 3.94E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

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CAS #: 000109-86-4 Name: 2-METHOXYETHANOL

```
*******************************************************************************
MELT     2-METHOXYETHANOL                                        CAS#   109-86-4
  Melting Point  :  -85.1        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP       2-METHOXYETHANOL                                        CAS#   109-86-4
  Vapor Pressure :  9.5          MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*******************************************************************************

VP       2-METHOXYETHANOL                                        CAS#   109-86-4
  Vapor Pressure :  9.01         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

DOW CHEMICAL COMPANY (1981)
DOW CHEMICAL COMPANY.; THE GLYCOL ETHERS HANDBOOK.; MIDLAND, MI: DOW CHEMICAL CO.; 1981

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

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CAS #: 000110-12-3 Name: 5-METHYL-2-HEXANONE

```
*****************************************************************************
MELT    5-METHYL-2-HEXANONE                                  CAS#   110-12-3
  Melting Point  :  -73.9        DEG C
  Remarks        :
            1    :  LEWIS (1993)
            2    :   HPV: METHYL ISOMYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************

VP      5-METHYL-2-HEXANONE                                  CAS#   110-12-3
  Vapor Pressure :  5.200E+00    MM HG        MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************

VP      5-METHYL-2-HEXANONE                                  CAS#   110-12-3
  Vapor Pressure :  5.77         MM HG        MEASURED
  Temperature (C):  25
  Remarks        :
            1    :  ALARIE (1995)
            2    :   HPV: METHYL ISOMYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

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CAS #: 000110-43-0 Name: 2-HEPTANONE

```
*****************************************************************************
MELT    2-HEPTANONE                                          CAS#   110-43-0
  Melting Point  :  -35.5       DEG C
  Remarks        :
             1   :  LIDE (1993)
             2   :   HPV: METHYL N-AMYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************

VP      2-HEPTANONE                                          CAS#   110-43-0
  Vapor Pressure :  2.73        MM HG       MEASURED
  Temperature (C):  25
  Remarks        :
             1   :  RANGE OF VALUES, 1.6 TO 3.86 MM HG
             2   :   HSDB (2001)
             3   :   HPV: METHYL N-AMYL KETONE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************


   US EPA (2004)
   U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY
   CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.;  WASHINGTON, DC:
   USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE
   HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search
```

CHEMFATE Search Results

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CAS #: 000110-54-3 Name: N-HEXANE

```
*****************************************************************************
VP      N-HEXANE                                          CAS#   110-54-3
  Vapor Pressure :  .5900E+02   .9700E+02   .1520E+03   .2310E+03   TORR
                    MEASURED
  Temperature (C):  5.0         15.0        25.0        35.0
  Abbrev. Ref.   :  ZWOLINSKI,BJ & WILHOIT,RC (1971)
*****************************************************************************

VP      N-HEXANE                                          CAS#   110-54-3
  Vapor Pressure :  1.513E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

ZWOLINSKI,BJ & WILHOIT,RC (1971)
ZWOLINSKI,B.J.; WILHOIT,R.C.; HANDBOOK OF VAPOR PRESSURES AND HEATS OF VAPORIZATON OF HYDROCARBONS AND RELATED COMPOUNDS.; API44-TRC101. COLLEGE STATION,TX: THERMODYNAMCS RESEARCH CENTER.; 1971

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000110-54-3
Chem Name  : N-HEXANE
Mol Formula: C6H14
Mol Weight : 86.18
Melting Pt : -95.3 deg C
Boiling Pt : 68.7 deg C
Water Solubility:
   Value : 9.5 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : MCAULIFFE,C (1966)
Log P (octanol-water):
   Value : 3.90
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 151 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BOUBLIK,T ET AL. (1984)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 1.8 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 5.61E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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```
CAS Number : 000110-62-3
Chem Name  : 1-PENTANAL
Mol Formula: C5H10O
Mol Weight : 86.14
Melting Pt : -91.5 deg C
Boiling Pt : 103 deg C
Water Solubility:
   Value : 1.17E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.31
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 26 mm Hg
   Temp  : 20 deg C
   Type  : EXP
   Ref   : FLICK,EW (1991)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000147 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BUTTERY,RG ET AL. (1969)
Atmospheric OH Rate Constant:
   Value : 2.85E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CAS #: 000110-80-5 Name: 2-ETHOXYETHANOL

```
*****************************************************************************
MELT    2-ETHOXYETHANOL                                        CAS#   110-80-5
  Melting Point  :  -100        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*****************************************************************************

VP      2-ETHOXYETHANOL                                        CAS#   110-80-5
  Vapor Pressure :  .18E 01     .55E 01     .10E 02     TORR        MEASURED
  Temperature (C):  10.         25.         37.
  Remarks        :  TAKEN FROM GRAPHS
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*****************************************************************************

VP      2-ETHOXYETHANOL                                        CAS#   110-80-5
  Vapor Pressure :  .4E 01      TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  HANN,RWJR & JENSEN,PA (1977)
*****************************************************************************

VP      2-ETHOXYETHANOL                                        CAS#   110-80-5
  Vapor Pressure :  5.63        MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  KELLOMAEKI,A (1985)
*****************************************************************************

VP      2-ETHOXYETHANOL                                        CAS#   110-80-5
  Vapor Pressure :  5.310E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

DOW CHEMICAL COMPANY (1981)
DOW CHEMICAL COMPANY.; THE GLYCOL ETHERS HANDBOOK.; MIDLAND, MI: DOW CHEMICAL CO.; 1981

HANN,RWJR & JENSEN,PA (1977)

HANN,R.W. JR.; JENSEN,P.A.; WATER QUALITY CHARACTERISTICS OF HAZARDOUS MATERIALS.; NTIS-PB-285946. TEXAS A&M UNIV., COLLEGE STATION ENVIRONMENTAL ENGINEERING DIV. 1751 PP.; 1977

KELLOMAEKI,A (1985)
KELLOMAEKI,A.; VAPOR PRESSURE OF ETHYLENE GLYCOL MONOETHYL ETHER AND SOME O ITS CHLORIDE SOLVATES.; ACTA CHEM. SCAND. SER. A.; 39:77-8.; 1985

End of Search

CHEMFATE Search Results

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CAS #: 000110-82-7 Name: CYCLOHEXANE

```
*****************************************************************************
MELT    CYCLOHEXANE                                          CAS#   110-82-7
  Melting Point  :  6.554       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CAMPBELL,ML (1980)
*****************************************************************************

VP      CYCLOHEXANE                                          CAS#   110-82-7
  Vapor Pressure :  .4750E+02   .9761E+02   .1848E+03   TORR        CALCULATED
  Temperature (C):  10.0        25.0        40.0
  Remarks        :  CALC FROM ANTOINE EQN
  Abbrev. Ref.   :  ZWOLINSKI,BJ & WILHOIT,RC (1971)
*****************************************************************************

VP      CYCLOHEXANE                                          CAS#   110-82-7
  Vapor Pressure :  96.86       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CHAO,J ET AL. (1983)
*****************************************************************************
```

CAMPBELL,ML (1980)
CAMPBELL,M.L.; HYDROCARBONS C1-C6 (CYLCOHEXANE); KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. NY,NY: WILEY-INTERSCIENCE. 12:931-7.; 1980

CHAO,J ET AL. (1983)
CHAO,J.; LIN,C.T.; CHUNG,T.H.; VAPOR PRESSURE OF COAL CHEMICALS.; J. PHYS. CHEM. REF. DATA.; 12:1033-63.; 1983

ZWOLINSKI,BJ & WILHOIT,RC (1971)
ZWOLINSKI,B.J.; WILHOIT,R.C.; HANDBOOK OF VAPOR PRESSURES AND HEATS OF VAPORIZATON OF HYDROCARBONS AND RELATED COMPOUNDS.; API44-TRC101. COLLEGE STATION,TX: THERMODYNAMCS RESEARCH CENTER.; 1971

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```
CAS Number : 000110-83-8
Chem Name  : CYCLOHEXENE
Mol Formula: C6H10
Mol Weight : 82.15
Melting Pt : -103.5 deg C
Boiling Pt : 82.9 deg C
Water Solubility:
   Value : 213 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 2.86
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 89 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0455 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HINE,J & MOOKERJEE,PK (1975)
Atmospheric OH Rate Constant:
   Value : 6.77E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000111-65-9
Chem Name  : OCTANE
Mol Formula: C8H18
Mol Weight : 114.23
Melting Pt : -56.8 deg C
Boiling Pt : 125.6 deg C
Water Solubility:
   Value : 0.66 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 5.18
   Type  : EXP
   Ref   : MILLER,MM ET AL. (1985)
Vapor Pressure:
   Value : 14.1 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YAWS,CL (1994)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.21 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 8.68E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CAS #: 000111-84-2 Name: NONANE

```
*******************************************************************************
VP      NONANE                                                  CAS#   111-84-2
  Vapor Pressure :  4.450E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000111-84-2
Chem Name  : N-NONANE
Mol Formula: C9H20
Mol Weight : 128.26
Melting Pt : -53.5 deg C
Boiling Pt : 150.8 deg C
Water Solubility:
   Value : 220 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 4.76
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 4.45 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.4 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.02E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

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CAS #: 000121-44-8 Name: TRIETHYLAMINE

```
*******************************************************************************
MELT    TRIETHYLAMINE                                          CAS#   121-44-8
  Melting Point  :  -115        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      TRIETHYLAMINE                                          CAS#   121-44-8
  Vapor Pressure :  57.07       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

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Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000123-19-3
Chem Name  : DI(N-PROPYL) KETONE
Mol Formula: C7H14O
Mol Weight : 114.19
Melting Pt : -33 deg C
Boiling Pt : 144 deg C
Water Solubility:
   Value : 3200 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.73
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 6.12 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 5.49E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 9.34E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000123-38-6 Name: PROPIONALDEHYDE

```
*******************************************************************************
MELT    PROPIONALDEHYDE                                          CAS#   123-38-6
  Melting Point  :  -80          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      PROPIONALDEHYDE                                          CAS#   123-38-6
  Vapor Pressure :  316.8        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

Data From SRC PhysProp Database:

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```
CAS Number : 000123-51-3
Chem Name  : ISOPENTANOL
Mol Formula: C5H12O
Mol Weight : 88.15
Melting Pt : -117.2 deg C
Boiling Pt : 131.1 deg C
Water Solubility:
   Value : 2.67E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 1.16
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 2.37 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 1.41E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BUTLER,JAV ET AL. (1935)
Atmospheric OH Rate Constant:
   Value : 1.31E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : SAUNDERS,SM ET AL. (1993)
```

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CHEMFATE Search Results

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CAS #: 000123-86-4 Name: N-BUTYL ACETATE

```
*****************************************************************************
VP      N-BUTYL ACETATE                                        CAS#   123-86-4
  Vapor Pressure :  .15E 02     TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  SYRACUSE RESEARCH CORP (1979)
*****************************************************************************

VP      N-BUTYL ACETATE                                        CAS#   123-86-4
  Vapor Pressure :  .10E 02     .15E 02     TORR        MEASURED
  Temperature (C):  20.         25.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*****************************************************************************

VP      N-BUTYL ACETATE                                        CAS#   123-86-4
  Vapor Pressure :  1.151E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

SYRACUSE RESEARCH CORP (1979)
SYRACUSE RESEARCH CORP.; INFORMATION PROFILES ON POTENTIAL OCCUPATIONAL HAZARDS. VOLUME I. SINGLE CHEMICALS.; CONTRACT NO. 210-78-0019. PREPARED F NIOSH. SYRACUSE,NY: SYRACUSE RESEARCH CORP.; 1979

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000123-86-4
Chem Name  : N-BUTYL ACETATE
Mol Formula: C6H12O2
Mol Weight : 116.16
Melting Pt : -78 deg C
Boiling Pt : 126.1 deg C
Water Solubility:
   Value : 8400 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.78
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 11.5 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000281 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KIECKBUSCH,TG & KING,CJ (1979)
Atmospheric OH Rate Constant:
   Value : 4.9E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

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CHEMFATE Search Results

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CAS #: 000123-91-1 Name: 1,4-DIOXANE

```
*******************************************************************************
MELT    1,4-DIOXANE                                          CAS#   123-91-1
  Melting Point  :  11.80       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      1,4-DIOXANE                                          CAS#   123-91-1
  Vapor Pressure :  38.09       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

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CAS #: 000126-98-7 Name: METHACRYLONITRILE

```
*******************************************************************************
VP      METHACRYLONITRILE                                    CAS#   126-98-7
  Vapor Pressure :  7.120E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000126-98-7
Chem Name  : METHACRYLONITRILE
Mol Formula: C4H5N
Mol Weight : 67.09
Melting Pt : -35.8 deg C
Boiling Pt : 90.3 deg C
Water Solubility:
   Value : 2.54E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.68
   Type  : EXP
   Ref   : TANII,H & HASHIMOTO,K (1984)
Vapor Pressure:
   Value : 71.2 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000247 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 8.36E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000127-19-5
Chem Name  : N,N'-DIMETHYLACETAMIDE
Mol Formula: C4H9NO
Mol Weight : 87.12
Melting Pt : -20 deg C
Boiling Pt : 165 deg C
Water Solubility:
   Value : 1E+006 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : -0.77
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 2 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 10.8
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Henry's Law Constant:
   Value : 1.31E-008 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : TAFT,RW ET AL. (1985)
Atmospheric OH Rate Constant:
   Value : 1.36E-011 cm3/molecule-sec
   Temp  : 27 deg C
   Type  : EXP
   Ref   : KOCH,R ET AL. (1997)
```

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CHEMFATE Search Results

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CAS #: 000141-78-6 Name: ETHYL ACETATE

```
*******************************************************************************
MELT    ETHYL ACETATE                                          CAS#   141-78-6
  Melting Point  :  -83.6       DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1985)
*******************************************************************************

VP      ETHYL ACETATE                                          CAS#   141-78-6
  Vapor Pressure :  .243E 02    .689E 02    .9450E 02   .1652E 03   TORR
                    MEASURED
  Temperature (C):  -.11        18.67       25.         37.06
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1981)
*******************************************************************************

VP      ETHYL ACETATE                                          CAS#   141-78-6
  Vapor Pressure :  93.66       MM HG
  Temperature (C):  25
  Remarks        :  CALCULATED FROM T-RANGE OF -83.4 TO 250.25 DEG C, SRC
                    RECOMMEDNED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

AMBROSE,D ET AL. (1981)
AMBROSE,D.; ELLENDER,J.H.; GUNDRY,H.A.; LEE,D.A.; TOWNSEND,R.; THERMODYNAMI PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. LI. THE VAPOUR PRESSURES OF SOME ESTERS AND FATTY ACIDS.; J. CHEM. THERM.; 13:795-802.; 1981

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

WEAST,RC ET AL. (1985)
WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS 66TH ED; CRC PRESS; BOCA RATON, FLA; 1985

End of Search

CHEMFATE Search Results

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CAS #: 000141-79-7 Name: MESITYL OXIDE

```
*******************************************************************************
VP      MESITYL OXIDE                                          CAS#   141-79-7
  Vapor Pressure :  1.102E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

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```
CAS Number : 000141-79-7
Chem Name  : MESITYL OXIDE
Mol Formula: C6H10O
Mol Weight : 98.15
Melting Pt : -59 deg C
Boiling Pt : 130 deg C
Water Solubility:
   Value : 2.89E+004 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.37
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 8.21 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.67E-005 atm-m3/mole
   Temp  : 20 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 7.86E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000142-82-5
Chem Name  : N-HEPTANE
Mol Formula: C7H16
Mol Weight : 100.21
Melting Pt : -90.6 deg C
Boiling Pt : 98.5 deg C
Water Solubility:
   Value : 3.4 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 4.66
   Type  : EXP
   Ref   : MILLER,MM ET AL. (1985)
Vapor Pressure:
   Value : 46 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 2 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 7.15E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

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CAS #: 001634-04-4 Name: METHYL TERT-BUTYL ETHER

```
*******************************************************************************
MELT     METHYL TERT-BUTYL ETHER                                CAS#  1634-04-4
  Melting Point  :  -109        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP       METHYL TERT-BUTYL ETHER                                CAS#  1634-04-4
  Vapor Pressure :  .251E 03    TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1976)
*******************************************************************************

VP       METHYL TERT-BUTYL ETHER                                CAS#  1634-04-4
  Vapor Pressure :  249         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

AMBROSE,D ET AL. (1976)
AMBROSE,D.; ELLENDER,J.H.; SPRAKE, C.H.S.; TOWNSEND, R.; THERMODYNAMIC PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. XLIII. VAPOR PRESSURES OF SOME ETHERS.; J. CHEM. THERMODYN.; 8:165-78.; 1976

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000287-92-3 Name: CYCLOPENTANE

```
*****************************************************************************
VP      CYCLOPENTANE                                          CAS#   287-92-3
  Vapor Pressure :  3.178E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000287-92-3
Chem Name  : CYCLOPENTANE
Mol Formula: C5H10
Mol Weight : 70.14
Melting Pt : -93.8 deg C
Boiling Pt : 49.3 deg C
Water Solubility:
   Value : 156 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 3.00
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 318 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.188 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 5.16E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 004170-30-3
Chem Name  : CROTONALDEHYDE
Mol Formula: C4H6O
Mol Weight : 70.09
Melting Pt : -76.5 deg C
Boiling Pt : 104 deg C
Water Solubility:
   Value : 1.81E+005 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : BAXTER,WFJR (1979)
Log P (octanol-water):
   Value : 0.60
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 30 mm Hg
   Temp  : 20 deg C
   Type  : EXP
   Ref   : WEBER,RC ET AL. (1981)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.68E-006 atm-m3/mole
   Temp  : 20 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.62E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000460-19-5 Name: CYANOGEN

```
*******************************************************************************
VP      CYANOGEN                                                CAS#   460-19-5
  Vapor Pressure :  4.302E+03   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000460-19-5
Chem Name  : CYANOGEN
Mol Formula: C2N2
Mol Weight : 52.04
Melting Pt : -27.9 deg C
Boiling Pt : -21.1 deg C
Water Solubility:
   Value : 1.51E+005 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.07
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 4300 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0054 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000050-00-0 Name: FORMALDEHYDE

```
*****************************************************************************
MELT     FORMALDEHYDE                                          CAS#     50-00-0
  Melting Point  :  -92          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1985)
*****************************************************************************

VP       FORMALDEHYDE                                          CAS#     50-00-0
  Vapor Pressure :  5.24E 03     MM HG        MEAS
  Temperature (C):  25
  Remarks        :  INTERPOLATED FROM DATA OBTAINED IN THE RANGE -92 TO 135 DE
                    C, SRC RECOMMENDED VALUE.
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

WEAST,RC ET AL. (1985)
WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS 66TH ED; CRC PRESS; BOCA RATON, FLA; 1985

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000540-84-1
Chem Name  : 2,2,4-TRIMETHYLPENTANE
Mol Formula: C8H18
Mol Weight : 114.23
Melting Pt : -107.3 deg C
Boiling Pt : 99.2 deg C
Water Solubility:
   Value : 2.44 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 4.09
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 49.3 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1991)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.04 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.68E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000563-80-4 Name: 3-METHYL-2-BUTANONE

```
*******************************************************************************
VP      3-METHYL-2-BUTANONE                                   CAS#   563-80-4
  Vapor Pressure :  5.220E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************

VP      3-METHYL-2-BUTANONE                                   CAS#   563-80-4
  Vapor Pressure :  52.2        MM HG       MEASURED
  Temperature (C):  25
  Remarks        :
             1   :  DAUBERT AND DANNER (1989)
             2   :   HPV: 2-BUTANONE, 3-METHYL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

Data From SRC PhysProp Database:

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```
CAS Number : 000563-80-4
Chem Name  : 3-METHYL-2-BUTANONE
Mol Formula: C5H10O
Mol Weight : 86.14
Melting Pt : -92 deg C
Boiling Pt : 94.3 deg C
Water Solubility:
   Value : 6.08E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.84
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 52.2 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.73E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 2.87E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LECALVE,S ET AL. (1998)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000591-78-6 Name: METHYL N-BUTYL KETONE

```
*******************************************************************************
VP      METHYL N-BUTYL KETONE                                   CAS#   591-78-6
  Vapor Pressure :  .1162E 02   .199E 02    .672E 02    TORR        MEASURED
  Temperature (C):  25.0        34.6        59.4
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1975)
*******************************************************************************
```

AMBROSE,D ET AL. (1975)
AMBROSE,D.; ELLENDER,J.H.; LEES,E.B.; SPRAKE,C.H.S.; TOWNSEND,R.;
THERMODYNAMIC PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. XXXVIII. VAPOUR
PRESSURES OF SOME ALIPHATIC KETONES.; J. CHEM. THERM.; 7:453-72.; 1975

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000591-78-6
Chem Name  : 2-HEXANONE
Mol Formula: C6H12O
Mol Weight : 100.16
Melting Pt : -55.5 deg C
Boiling Pt : 127.6 deg C
Water Solubility:
   Value : 1.75E+004 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : PAPA,AJ & SHERMAN,PDJR (1981)
Log P (octanol-water):
   Value : 1.38
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 11.6 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : AMBROSE,D ET AL. (1975)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.32E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 9.1E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000060-29-7 Name: ETHYL ETHER

```
*******************************************************************************
VP      ETHYL ETHER                                          CAS#    60-29-7
  Vapor Pressure :  .4420E 03   TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  HANN,RWJR & JENSEN,PA (1977)
*******************************************************************************

VP      ETHYL ETHER                                          CAS#    60-29-7
  Vapor Pressure :  .442E 03    .921E 03    TORR        MEASURED
  Temperature (C):  20.         40.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*******************************************************************************

VP      ETHYL ETHER                                          CAS#    60-29-7
  Vapor Pressure :  5.371E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

HANN,RWJR & JENSEN,PA (1977)
HANN,R.W. JR.; JENSEN,P.A.; WATER QUALITY CHARACTERISTICS OF HAZARDOUS MATERIALS.; NTIS-PB-285946. TEXAS A&M UNIV., COLLEGE STATION ENVIRONMENTAL ENGINEERING DIV. 1751 PP.; 1977

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000060-29-7
Chem Name  : DIETHYL ETHER
Mol Formula: C4H10O
Mol Weight : 74.12
Melting Pt : -116.3 deg C
Boiling Pt : 34.5 deg C
Water Solubility:
   Value : 6.04E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 0.89
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 538 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1995)
pKa Dissociation Constant:
   Value : -3.59
   Temp  :
   Type  : EXP
   Ref   : KULEVSKY,N ET AL. (1969)
Henry's Law Constant:
   Value : 0.00123 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BOCEK,K (1976)
Atmospheric OH Rate Constant:
   Value : 1.31E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1994)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000060-35-5 Name: ACETAMIDE

```
*****************************************************************************
MELT    ACETAMIDE                                          CAS#    60-35-5
  Melting Point  :  69.5        DEGC
  Remarks        :  SRC RECOMMENDED VALUE, 80 DEG C FREEZING POINT (RIDDICK,J
                    AL. (1986)
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ACETAMIDE                                          CAS#    60-35-5
  Vapor Pressure :  0.11        MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED USING PCCHEM, BASED ON BP = 221 DEG C FROM MERCK
                    INDEX (1983), SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************
```

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI
AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY
WILEY-INTERSCIENCE. 2:PP.1325; 1986

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000624-83-9 Name: METHYLISOCYANATE

```
*******************************************************************************
MELT    METHYLISOCYANATE                                        CAS#   624-83-9
  Melting Point  :  -45          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1985)
*******************************************************************************

VP      METHYLISOCYANATE                                        CAS#   624-83-9
  Vapor Pressure :  221          MM HG
  Temperature (C):  25
  Remarks        :  EST USING METHOD IN NEELY,WB & BLAU,GE (1985), SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      METHYLISOCYANATE                                        CAS#   624-83-9
  Vapor Pressure :  3.480E+02    MM HG        MEASURED
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  UNION CARBIDE (1979)
*******************************************************************************


   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

   UNION CARBIDE (1979)
   UNION CARBIDE; 1979-1980 CHEMICALS AND PLASTICS PHYSICAL PROPERTIES.;  UNIO
   CARBIDE CORP., NEW YORK. P. 17.; 1979

   WEAST,RC ET AL. (1985)
   WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS
   66TH ED;  CRC PRESS; BOCA RATON, FLA; 1985

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000064-17-5 Name: ETHANOL

```
*******************************************************************************
MELT    ETHANOL                                                CAS#    64-17-5
  Melting Point  :  -114.49      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

MELT    ETHANOL                                                CAS#    64-17-5
  Melting Point  :  -114         DEG C
  Remarks        :
             1   :  VERSCHUEREN (1996)
             2   :   HPV: ETHANOL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************

VP      ETHANOL                                                CAS#    64-17-5
  Vapor Pressure :  59.26        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************

VP      ETHANOL                                                CAS#    64-17-5
  Vapor Pressure :  59.03        MM HG        MEASURED
  Temperature (C):  25
  Remarks        :
             1   :  USED EQUILIBRIUM STILL OF SCATCHARD ET AL. METHOD
             2   :   KRETSCHMER ET AL. (1948)
             3   :   HPV: ETHANOL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC:

USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000064-18-6 Name: FORMIC ACID

```
*******************************************************************************
MELT    FORMIC ACID                                          CAS#    64-18-6
  Melting Point  :  8.27        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      FORMIC ACID                                          CAS#    64-18-6
  Vapor Pressure :  42.59       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000064-19-7 Name: ACETIC ACID

```
*****************************************************************************
VP      ACETIC ACID                                          CAS#    64-19-7
  Vapor Pressure :  .156E 02    .2168E 02   .3780E 02   .6635E 02   TORR
                    MEASURED
  Temperature (C):  25.0        30.9        41.5        53.1
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1977)
*****************************************************************************

VP      ACETIC ACID                                          CAS#    64-19-7
  Vapor Pressure :  .114E 02    .20E 02     TORR        MEASURED
  Temperature (C):  20.         30.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*****************************************************************************

VP      ACETIC ACID                                          CAS#    64-19-7
  Vapor Pressure :  1.573E+01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************

VP      ACETIC ACID                                          CAS#    64-19-7
  Vapor Pressure :  11.4        MM HG       MEASURED
  Temperature (C):  20
  Remarks        :
            1    :  VERSCHUEREN (1996)
            2    :   HPV: ACETIC ACID AND SALTS.
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************
```

AMBROSE,D ET AL. (1977)
AMBROSE,D.; ELLENDER,J.H.; SPRAKE,C.H.S.; TOWNSEND,R.; THERMODYNAMIC PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. XLV. THE VAPOUR PRESSURE OF ACETIC ACID.; J. CHEM. THERM.; 9:735-41.; 1977

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE

HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000064-19-7
Chem Name  : ACETIC ACID
Mol Formula: C2H4O2
Mol Weight : 60.05
Melting Pt : 16.6 deg C
Boiling Pt : 117.9 deg C
Water Solubility:
   Value : 1E+006 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : MERCK INDEX (1996)
Log P (octanol-water):
   Value : -0.17
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 15.7 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value : 4.76
   Temp  : 25 deg C
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 1E-007 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : GAFFNEY,JS ET AL. (1987)
Atmospheric OH Rate Constant:
   Value : 7.4E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000067-56-1 Name: METHANOL

```
*******************************************************************************
MELT    METHANOL                                                  CAS#    67-56-1
  Melting Point  :  -97.68      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

MELT    METHANOL                                                  CAS#    67-56-1
  Melting Point  :  -97.8       DEG C
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      METHANOL                                                  CAS#    67-56-1
  Vapor Pressure :  127         MM HG       MEAS
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      METHANOL                                                  CAS#    67-56-1
  Vapor Pressure :  126         MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************

VP      METHANOL                                                  CAS#    67-56-1
  Vapor Pressure :  95          MM HG       MEASURED
  Temperature (C):  25
  Remarks        :
            1    :  BOUBLICK ET AL. (1984)
            2    :   HPV: METHANOL.
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK,

NY., 4 VOL.; 1989

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000067-63-0 Name: ISOPROPANOL

```
*****************************************************************************
MELT    ISOPROPANOL                                          CAS#    67-63-0
  Melting Point  :  -88.0       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ISOPROPANOL                                          CAS#    67-63-0
  Vapor Pressure :  45.42       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Acetone
CAS Number: 000067-64-1

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	9.0E-1	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	5.3E+3	mg/kg	ACGIH
Dermal LD50:	2.0E+4	mg/kg	ACGIH
Gas Inhal LC50:		ppm	
Dust Inhal LC50:	3.7E+1	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.0E+4	µg/L	ECOTOX
Salt Ecol LC50:	1.9E+6	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.2E+0	days	THOMAS
Photolysis:	5.7E-1	days	CHEMFATE
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.2E+0	days	THOMAS
Photolysis:	5.7E-1	days	CHEMFATE
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
Log Kow:	-2.4E-1		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	5.8E+1	
Density:	7.9E-1	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.3E+2	Torr	CHEMFATE
Henry's Law:	3.9E-5	atm-m3/mol	CHEMFATE
Water Solub:	1.0E+6	mg/L	CHEMFATE
Distrib Coef:	8.7E-2	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	-2.4E-1		CHEMFATE
Water Solub:	1.0E+6		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-9.5E+1	C
Boiling Point:	5.6E+1	C
Formula:	C3 H6 O	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000067-64-1 Name: ACETONE

```
*****************************************************************************
MELT    ACETONE                                                CAS#    67-64-1
  Melting Point  :  -94.7       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ACETONE                                                CAS#    67-64-1
  Vapor Pressure :  231.5       MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************

VP      ACETONE                                                CAS#    67-64-1
  Vapor Pressure :  230.0       MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

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BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000071-23-8 Name: N-PROPANOL

```
*******************************************************************************
MELT     N-PROPANOL                                          CAS#     71-23-8
  Melting Point  :  -127        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP       N-PROPANOL                                          CAS#     71-23-8
  Vapor Pressure :  20.99       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************
```

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End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000071-36-3 Name: 1-BUTANOL

```
*******************************************************************************
MELT    1-BUTANOL                                          CAS#    71-36-3
  Melting Point  :  -88.62      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      1-BUTANOL                                          CAS#    71-36-3
  Vapor Pressure :  .103E 01    .234E 01    .502E 01    .1006E 02   .1933E 02
                    .3539E 02   TORR        MEASURED
  Temperature (C):  0.0         10.0        20.0        30.0        40.0
                    50.2
  Abbrev. Ref.   :  MUNDAY,EB ET AL. (1980)
*******************************************************************************

VP      1-BUTANOL                                          CAS#    71-36-3
  Vapor Pressure :  .471E 01    TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  SHERMAN,PDJR (1978)
*******************************************************************************

VP      1-BUTANOL                                          CAS#    71-36-3
  Vapor Pressure :  6.7         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      1-BUTANOL                                          CAS#    71-36-3
  Vapor Pressure :  7.00        MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

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MUNDAY,EB ET AL. (1980)
MUNDAY,E.B.; MULLINS,J.C.; EDIE,D.D.; VAPOR PRESSURE DATA FOR TOLUENE, 1-PENTANOL, 1-BUTANOL, WATER, AND 1-PROPANOL AND FOR THE WATER AND 1-PROPAN SYSTEM FROM 273.15 TO 323.15.; J. CHEM. ENG. DATA.; 25:191-4.; 1980

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End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000074-99-7
Chem Name  : PROPYNE
Mol Formula: C3H4
Mol Weight : 40.07
Melting Pt : -102.7 deg C
Boiling Pt : -23.2 deg C
Water Solubility:
   Value : 3640 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : MCAULIFFE,C (1966)
Log P (octanol-water):
   Value : 0.94
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 4310 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.011 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 5.9E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-05-8 Name: ACETONITRILE

```
*****************************************************************************
MELT    ACETONITRILE                                        CAS#    75-05-8
  Melting Point  :  -45          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP      ACETONITRILE                                        CAS#    75-05-8
  Vapor Pressure :  .5490E+02   .7090E+02   .1106E+03   TORR        MEASURED
  Temperature (C):  15.5        20.         30.
  Abbrev. Ref.   :  BEILSTEIN (NA--)
*****************************************************************************

VP      ACETONITRILE                                        CAS#    75-05-8
  Vapor Pressure :  88.8        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************

VP      ACETONITRILE                                        CAS#    75-05-8
  Vapor Pressure :  91.1        MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

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MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-07-0 Name: ACETALDEHYDE

```
*****************************************************************************
MELT    ACETALDEHYDE                                          CAS#    75-07-0
  Melting Point  :  -123        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ACETALDEHYDE                                          CAS#    75-07-0
  Vapor Pressure :  .3300E+03   .5080E+03   .7545E+03   TORR        MEASURED
  Temperature (C):  0.0         10.0        20.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  HAGEMEYER,HJ (1978)
*****************************************************************************

VP      ACETALDEHYDE                                          CAS#    75-07-0
  Vapor Pressure :  902         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

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End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-12-7 Name: FORMAMIDE

```
*******************************************************************************
MELT    FORMAMIDE                                          CAS#    75-12-7
  Melting Point  :  2.55        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  EBERLING,CL (1980)
*******************************************************************************

VP      FORMAMIDE                                          CAS#    75-12-7
  Vapor Pressure :  .98E 00     .200E 02    .9998E 02   TORR        MEASURED
  Temperature (C):  70.5        122.5       157.5
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  EBERLING,CL (1981)
*******************************************************************************

VP      FORMAMIDE                                          CAS#    75-12-7
  Vapor Pressure :  0.023       MM HG
  Temperature (C):  25
  Remarks        :
             1   :  EXTRAPOLATED FROM REPORTED ANTOINNE'S EQUATION IN RIDDICK,
                    ET AL (1986)
             2   :   EXPERIMENTAL TEMPERATURE RANGE OF EQUATION NOT REPORTED,
                    SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      FORMAMIDE                                          CAS#    75-12-7
  Vapor Pressure :  6.100E-02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

EBERLING,CL (1980)
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11:258-63; 1981

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End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Carbon disulfide
CAS Number: 000075-15-0

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	1.0E-1	mg/kg/day	IRIS
Inhal RfD:	2.0E-1	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	1.2E+3	mg/kg	RTECS
Dermal LD50:		mg/kg	
Gas Inhal LC50:	2.0E+3	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.9E+3	µg/L	ECOTOX
Salt Ecol LC50:	4.5E+4	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	4.0E+2	days	CHEMFATE
Volatility:	7.7E+1	days	THOMAS
Photolysis:	1.1E+1	days	CHEMFATE
Biodeg:		days	
Radio:		days	
RIVER - Halflives			
Hydrolysis:	4.0E+2	days	CHEMFATE
Volatility:	8.3E-1	days	THOMAS
Photolysis:	1.1E+1	days	CHEMFATE
Biodeg:		days	
Radio:		days	
Log Kow:	2.2E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	No	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	7.6E+1	
Density:	1.3E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	3.6E+2	Torr	CHEMFATE
Henry's Law:	3.0E-2	atm-m3/mol	CHEMFATE
Water Solub:	1.2E+3	mg/L	CHEMFATE
Distrib Coef:	9.1E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.2E+0		CHEMFATE
Water Solub:	1.2E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-1.2E+2	C
Boiling Point:	4.6E+1	C
Formula:	C S2	

CLASS INFORMATION

Class	Parent Substance

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About SRC Locations Business Areas Career Center Training

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-15-0 Name: CARBON DISULFIDE

```
*******************************************************************************
MELT    CARBON DISULFIDE                                        CAS#    75-15-0
  Melting Point  :  46.2        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      CARBON DISULFIDE                                        CAS#    75-15-0
  Vapor Pressure :  .1270E+03   .2970E+03   .7580E+03   TORR        MEASURED
  Temperature (C):  0.0         20.0        46.3
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  TIMMERMAN,RW (1978)
*******************************************************************************

VP      CARBON DISULFIDE                                        CAS#    75-15-0
  Vapor Pressure :  358         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      CARBON DISULFIDE                                        CAS#    75-15-0
  Vapor Pressure :  359         MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
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End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-21-8 Name: ETHYLENE OXIDE

```
*******************************************************************************
MELT    ETHYLENE OXIDE                                          CAS#    75-21-8
  Melting Point  :  -111        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      ETHYLENE OXIDE                                          CAS#    75-21-8
  Vapor Pressure :  .1095E 04   TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  MARTIN,H & WORTHING,CR (1977)
*******************************************************************************

VP      ETHYLENE OXIDE                                          CAS#    75-21-8
  Vapor Pressure :  .116E 04    TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  GALLANT,RW (1967)
*******************************************************************************

VP      ETHYLENE OXIDE                                          CAS#    75-21-8
  Vapor Pressure :  .1305E 04   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  BOGYO,DA ET AL. (1980)
*******************************************************************************

VP      ETHYLENE OXIDE                                          CAS#    75-21-8
  Vapor Pressure :  .7791E 03   TORR        MEASURED
  Temperature (C):  11.06
  Abbrev. Ref.   :  MCDONALD,RA ET AL. (1959)
*******************************************************************************

VP      ETHYLENE OXIDE                                          CAS#    75-21-8
  Vapor Pressure :  1314        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

BOGYO,DA ET AL. (1980)
BOGYO,D.A.; LANDE,S.S.; MEYLEN,W.M.; HOWARD,P.H.; SANTODONATO,J.;
INVESTIGATION OF SELECTED ENVIRONMENTAL CONTAMINANTS: EPOXIDES.;
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GALLANT,RW (1967)
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MARTIN,H.; WORTHING,C.R.; PESTICIDE MANUAL. FIFTH EDITION, BRITISH CROP PROTECTION COUNCIL. 563 PP.; 1977

MCDONALD,RA ET AL. (1959)
MCDONALD,R.A.; SHRADER,S.A.; STULL,D.R.; VAPOR PRESSURES AND FREEZING POINT OF 30 ORGANICS.; J. CHEM. ENG. DATA.; 4:311-13.; 1959

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-44-5 Name: PHOSGENE

```
*****************************************************************************
MELT     PHOSGENE                                          CAS#     75-44-5
  Melting Point   :  -118        DEGC
  Remarks         :  SRC RECOMMENDED VALUE
  Abbrev. Ref.    :  MERCK INDEX (1983)
*****************************************************************************

VP       PHOSGENE                                          CAS#     75-44-5
  Vapor Pressure  :  0.5566E 03  0.8155E 03  0.9940E 03  0.1222E 04  0.1485E 04
                     TORR        MEASURED
  Temperature (C) :  0.0         9.6         15.0        20.9        26.7
  Abbrev. Ref.    :  GERMANN,AFO & TAYLOR,QW (1926)
*****************************************************************************

VP       PHOSGENE                                          CAS#     75-44-5
  Vapor Pressure  :  1418        MM HG
  Temperature (C) :  25
  Remarks         :  SRC RECOMMENDED VALUE
  Abbrev. Ref.    :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

GERMANN,AFO & TAYLOR,QW (1926)
GERMANN,A.F.O.; TAYLOR,Q.W.; THE CRITICAL CONSTANTS AND VAPOR TENSION OF PHOSSGENE.; J. AM. CHEM. SOC.; 48:11554-9.; 1926

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-50-3 Name: TRIMETHYL AMINE

```
*******************************************************************************
MELT    TRIMETHYL AMINE                                          CAS#    75-50-3
  Melting Point  :  -124        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      TRIMETHYL AMINE                                          CAS#    75-50-3
  Vapor Pressure :  .1432E 04   TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  SCHWEIZER,AE ET AL. (1978)
*******************************************************************************

VP      TRIMETHYL AMINE                                          CAS#    75-50-3
  Vapor Pressure :  1607        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

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SCHWEIZER,AE ET AL. (1978)
SCHWEIZER,A.E.; FOWLKES,R.L.; MCMAKIN,J.H.; WHYTE,T.E. JR.; AMINES (LOWER ALIPHATIC).; IN: KIRK-OTHMER ENCYCL. CHEM. TECHNOL. 3RD ED. 2:272-83.; 197

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000075-52-5
Chem Name  : NITROMETHANE
Mol Formula: CH3NO2
Mol Weight : 61.04
Melting Pt : -28.5 deg C
Boiling Pt : 101.1 deg C
Water Solubility:
   Value : 1.11E+005 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : -0.35
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 35.8 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 10.2
   Temp  : 25 deg C
   Type  :
   Ref   : RIDDICK,JA ET AL. (1986)
Henry's Law Constant:
   Value : 2.86E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : GAFFNEY,JS ET AL. (1987)
Atmospheric OH Rate Constant:
   Value : 1.3E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-55-8 Name: 2-METHYLAZIRIDINE

```
*******************************************************************************
MELT    2-METHYLAZIRIDINE                                        CAS#    75-55-8
  Melting Point  :  -65.00      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HAM,GE (1981)
*******************************************************************************

VP      2-METHYLAZIRIDINE                                        CAS#    75-55-8
  Vapor Pressure :  111.8       MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HAM,GE (1981)
*******************************************************************************


   HAM,GE (1981)
   HAM,GE; IMINES, CYCLIC.;  KIRK-OTHMER ENCYCL CHEM TECH 3RD ED. NY,NY:
   WILEY-INTERSCIENCE. 13:142-66; 1981

End of Search
```

Syracuse Research Corporation

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000075-65-0 Name: TERT-BUTANOL

```
*****************************************************************************
MELT     TERT-BUTANOL                                          CAS#     75-65-0
  Melting Point   :  25.62        DEGC
  Remarks         :  SRC RECOMMENDED VALUE
  Abbrev. Ref.    :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP       TERT-BUTANOL                                          CAS#     75-65-0
  Vapor Pressure :  .306E 02     TORR         MEASURED
  Temperature (C):  20.
  Remarks         :  UNITS CONVERTED
  Abbrev. Ref.    :  SHERMAN,PDJR (1978)
*****************************************************************************

VP       TERT-BUTANOL                                          CAS#     75-65-0
  Vapor Pressure :  41.7         MM HG
  Temperature (C):  25
  Remarks         :  EXTRAPOLATED FROM DATA BEGINNING AT 39.15 DEG C, SRC
                     RECOMMENDED VALUE
  Abbrev. Ref.    :  BOUBLIK,T ET AL. (1984)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PRCPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

SHERMAN,PDJR (1978)
SHERMAN,P.D. JR.; BUTYL ALCOHOLS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECHNOL. 3RD ED. 4:338-45.; 1978

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000765-34-4 Name: GLYCIDYLALDEHYDE

```
*******************************************************************************
MELT    GLYCIDYLALDEHYDE                                        CAS#   765-34-4
  Melting Point  :  -62          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DEAN,JA (1985)
*******************************************************************************

VP      GLYCIDYLALDEHYDE                                        CAS#   765-34-4
  Vapor Pressure :  27           MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************


   DEAN,JA (1985)
   DEAN,J.A.; LANGE'S HANDBOOK OF CHEMISTRY 13TH ED.;  NY, NY: MCGRAW-HILL BOO
   CO.; 1985

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000078-83-1 Name: ISOBUTYL ALCOHOL

```
*****************************************************************************
MELT    ISOBUTYL ALCOHOL                                        CAS#    78-83-1
  Melting Point  :  -108        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ISOBUTYL ALCOHOL                                        CAS#    78-83-1
  Vapor Pressure :  .126E 02    TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  DORIGAN,J ET AL. (1976)
*****************************************************************************

VP      ISOBUTYL ALCOHOL                                        CAS#    78-83-1
  Vapor Pressure :  .880E 01    TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  SHERMAN,PDJR (1978)
*****************************************************************************

VP      ISOBUTYL ALCOHOL                                        CAS#    78-83-1
  Vapor Pressure :  10.45       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

DORIGAN,J ET AL. (1976)
DORIGAN,J.; FULLER,B.; DUFFY,R.; PRELIMINARY SCORING OF SELECTED ORGANIC AI POLLUTANTS. APPENDIX III-CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS F THROUGH N.; EPA-450/3-77-008D. RESEARCH TRIANGLE PARK,NC: U.S. EPA. PP.303 1976

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

SHERMAN,PDJR (1978)
SHERMAN,P.D. JR.; BUTYL ALCOHOLS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECHNOL.

3RD ED. 4:338-45.; 1978

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000078-92-2 Name: 2-BUTANOL

```
*******************************************************************************
MELT    2-BUTANOL                                          CAS#    78-92-2
  Melting Point  :  -114.7      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      2-BUTANOL                                          CAS#    78-92-2
  Vapor Pressure :  18.33       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Methyl ethyl ketone

CAS Number: 000078-93-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	6.0E-1	mg/kg/day	IRIS
Inhal RfD:	1.4E+0	mg/kg/day	IRIS
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	5.5E+3	mg/kg	ACGIH
Dermal LD50:	6.5E+3	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:	2.7E+4	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	5.2E+5	µg/L	ECOTOX
Salt Ecol LC50:	4.0E+5	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	1.8E+4	days	FATERATE
Volatility:	7.5E+1	days	THOMAS
Photolysis:		days	
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	1.8E+4	days	FATERATE
Volatility:	1.2E+0	days	THOMAS
Photolysis:		days	
Biodeg:	7.0E+0	days	FATERATE
Radio:		days	
Log Kow:	2.9E-1		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	7.2E+1	
Density:	8.0E-1	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	9.5E+1	Torr	CHEMFATE
Henry's Law:	5.6E-5	atm-m3/mol	CHEMFATE
Water Solub:	2.2E+5	mg/L	CHEMFATE
Distrib Coef:	2.9E-1	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.9E-1		CHEMFATE
Water Solub:	2.2E+5		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-8.7E+1	C
Boiling Point:	8.0E+1	C
Formula:	C4 H8 O	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000078-93-3 Name: METHYL ETHYL KETONE

```
*******************************************************************************
MELT    METHYL ETHYL KETONE                                    CAS#    78-93-3
  Melting Point  :  -86          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      METHYL ETHYL KETONE                                    CAS#    78-93-3
  Vapor Pressure :  95.3         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-09-4 Name: PROPIONIC ACID

```
*******************************************************************************
MELT     PROPIONIC ACID                                          CAS#     79-09-4
  Melting Point  :  -20.8        DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SAX,NI & LEWIS,RJSR (1987)
*******************************************************************************

VP       PROPIONIC ACID                                          CAS#     79-09-4
  Vapor Pressure :  .29E 01      TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*******************************************************************************

VP       PROPIONIC ACID                                          CAS#     79-09-4
  Vapor Pressure :  .338E 01     .2168E 02   TORR        MEASURED
  Temperature (C):  25.0         55.1
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1981)
*******************************************************************************

VP       PROPIONIC ACID                                          CAS#     79-09-4
  Vapor Pressure :  3.53         MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

AMBROSE,D ET AL. (1981)
AMBROSE,D.; ELLENDER,J.H.; GUNDRY,H.A.; LEE,D.A.; TOWNSEND,R.; THERMODYNAMI PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. LI. THE VAPOUR PRESSURES OF SOME ESTERS AND FATTY ACIDS.; J. CHEM. THERM.; 13:795-802.; 1981

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

SAX,NI & LEWIS,RJSR (1987)
SAX,N.I.; LEWIS,R.J.S.R.; HAWLEY'S CONDENSED CHEMICAL DICTIONARY 11TH ED; VANNOSTRAND REINHOLD CO.; N.Y.,N.Y.:P496; 1987

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-20-9 Name: METHYL ACETATE

```
*******************************************************************************
MELT    METHYL ACETATE                                          CAS#    79-20-9
  Melting Point  :  -98.1       DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1988)
*******************************************************************************

VP      METHYL ACETATE                                          CAS#    79-20-9
  Vapor Pressure :  216.2       MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  AMBROSE,D ET AL. (1981)
*******************************************************************************
```

AMBROSE,D ET AL. (1981)
AMBROSE,D.; ELLENDER,J.H.; GUNDRY,H.A.; LEE,D.A.; TOWNSEND,R.; THERMODYNAMI PROPERTIES OF ORGANIC OXYGEN COMPOUNDS. LI. THE VAPOUR PRESSURES OF SOME ESTERS AND FATTY ACIDS.; J. CHEM. THERM.; 13:795-802.; 1981

WEAST,RC ET AL. (1988)
WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS. 69TH ED.; BOCA RATON, FL: CRC PRESS INC.; 1988

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000080-62-6 Name: METHYL METHACRYLATE

```
*****************************************************************************
VP      METHYL METHACRYLATE                                  CAS#    80-62-6
  Vapor Pressure :  .83E 01     .293E 02    .810E 02    TORR        MEASURED
  Temperature (C):  0.          20.         40.
  Abbrev. Ref.   :  NEMEC,JW & KIRSCH,LS (1981)
*****************************************************************************

VP      METHYL METHACRYLATE                                  CAS#    80-62-6
  Vapor Pressure :  38.4        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

NEMEC,JW & KIRSCH,LS (1981)
NEMEC,J.W.; KIRSCH,L.S.; METHACRYLIC ACID AND DERIVATIVES.; IN: KIRK-OTHME ENCYCL. CHEM. TECHNOL. 3RD. ED. 15:346-76.; 1981

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000080-62-6
Chem Name  : METHYL METHACRYLATE
Mol Formula: C5H8O2
Mol Weight : 100.12
Melting Pt : -48 deg C
Boiling Pt : 100.5 deg C
Water Solubility:
   Value : 1.5E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : NEMEC,JW & KIRSCH,LS (1981)
Log P (octanol-water):
   Value : 1.38
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 38.5 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000319 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 2.6E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : SAUNDERS,SM ET AL. (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000096-22-0
Chem Name  : 3-PENTANONE
Mol Formula: C5H10O
Mol Weight : 86.14
Melting Pt : -39 deg C
Boiling Pt : 101.9 deg C
Water Solubility:
   Value : 4.81E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.99
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 37.7 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 8.88E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 2E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000097-63-2 Name: ETHYL METHACRYLATE

```
*******************************************************************************
MELT    ETHYL METHACRYLATE                                      CAS#    97-63-2
  Melting Point  :  -44.7       DEGC
  Remarks        :  ESTIMATED BY EQUATION 20 IN NEELY,WB & BLAU,GE (1985), SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      ETHYL METHACRYLATE                                      CAS#    97-63-2
  Vapor Pressure :  20.59       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************


   DAUBERT,TE & DANNER,RP (1985)
   DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE
   COMPOUNDS.;  AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000098-51-1 Name: P-TERT-BUTYLTOLUENE

```
*******************************************************************************
VP      P-TERT-BUTYLTOLUENE                                  CAS#    98-51-1
  Vapor Pressure :  .6710E 00   TORR        CALCULATED
  Temperature (C):  25.
  Abbrev. Ref.   :  DREISBACH,RR (1955)
*******************************************************************************
```

DREISBACH,RR (1955)
DREISBACH,R.R.; PHYSICAL PROPERTIES OF CHEMICAL COMPOUNDS. I.; ADVANCES IN CHEMISTRY SERIES NO. 15.; WASHINGTON, DC: AMERICAN CHEMICAL SOCIETY.; 1955

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000098-51-1
Chem Name  : P-(T-BUTYL)TOLUENE
Mol Formula: C11H16
Mol Weight : 148.25
Melting Pt : -52 deg C
Boiling Pt : 190 deg C
Water Solubility:
   Value : 5.5 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : AMOORE,JE & HAUTALA,E (1983)
Log P (octanol-water):
   Value : 5.17
   Type  : EXP
   Ref   : CHEM INSPECT TEST INST (1992)
Vapor Pressure:
   Value : 0.671 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : DREISBACH,RR (1955)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0154 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.4E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BOLZACCHINI,E ET AL. (1997)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000099-87-6 Name: P-CYMENE

```
*******************************************************************************
VP      P-CYMENE                                              CAS#    99-87-6
  Vapor Pressure :  1.460E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000099-87-6
Chem Name  : P-CYMENE
Mol Formula: C10H14
Mol Weight : 134.22
Melting Pt : -68.9 deg C
Boiling Pt : 177.1 deg C
Water Solubility:
   Value : 23.4 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BANERJEE,S ET AL (1980)
Log P (octanol-water):
   Value : 4.10
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 1.46 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.011 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.51E-011 cm3/molecule-sec
   Temp  : 22 deg C
   Type  : EXP
   Ref   : CORCHNOY,SB & ATKINSON,R (1990)
```

Back To PhysProp Demo Page

WTP RISK ASSESSMENT WORK PLAN IDENTIFIED CONSTITUENTS OF POTENTIAL CONCERN (COPC) SUPPORT DATA

Non-metals and Anions (NMA)

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 024959-67-9
Chem Name  : BROMIDE
Mol Formula: HBr
Mol Weight : 80.92
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 3.8E+004 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 0.63
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 7.94E-009 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0245 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000057-12-5
Chem Name  : CYANIDE ION
Mol Formula: CN
Mol Weight : 26.02
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 9.54E+004 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : -0.69
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 308 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0242 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 3E-014 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 007553-56-2
Chem Name  : IODINE
Mol Formula: I2
Mol Weight : 253.81
Melting Pt : 113.6 deg C
Boiling Pt : 185.24 deg C
Water Solubility:
   Value : 330 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : CLAYTON,GD & CLAYTON,FE (1994)
Log P (octanol-water):
   Value : 2.49
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.233 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LYDAY,PA (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0245 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 007647-01-0 Name: HYDROCHLORIC ACID

```
*******************************************************************************
VP      HYDROCHLORIC ACID                                    CAS#  7647-01-0
  Vapor Pressure :  3.540E+04   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 007664-39-3 Name: HYDROGEN FLUORIDE

```
*******************************************************************************
VP      HYDROGEN FLUORIDE                                        CAS#  7664-39-3
  Vapor Pressure :  9.172E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 007664-39-3
Chem Name  : HYDROGEN FLUORIDE
Mol Formula: HF
Mol Weight : 20.01
Melting Pt : -83.36 deg C
Boiling Pt : 20 deg C
Water Solubility:
   Value : 922 mg/L
   Temp  : 0 deg C
   Type  : EXP
   Ref   : DEAN,JA (1985)
Log P (octanol-water):
   Value : 0.23
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 917 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 3.19
   Temp  :
   Type  : EXP
   Ref   : BUDAVARI,S ET AL. (1996)
Henry's Law Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 007664-41-7 Name: AMMONIA

```
*****************************************************************************
VP      AMMONIA                                          CAS#  7664-41-7
  Vapor Pressure :  7.508E+03   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 007664-41-7
Chem Name  : AMMONIA
Mol Formula: H3N
Mol Weight : 17.03
Melting Pt : -77.7 deg C
Boiling Pt : -33.35 deg C
Water Solubility:
   Value : 4.82E+005 mg/L
   Temp  : 24 deg C
   Type  : EXP
   Ref   : DEAN,JA (1985)
Log P (octanol-water):
   Value : 0.23
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 7510 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 9.25
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LIDE,DR (1996)
Henry's Law Constant:
   Value : 1.61E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BETTERTON,EA (1992A)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 007782-50-5 Name: CHLORINE

```
*******************************************************************************
VP      CHLORINE                                                CAS#  7782-50-5
  Vapor Pressure :  5.854E+03   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 007782-50-5
Chem Name  : CHLORINE
Mol Formula: Cl2
Mol Weight : 70.91
Melting Pt : -101 deg C
Boiling Pt : -34.05 deg C
Water Solubility:
   Value : 6300 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : AMOORE,JE & HAUTALA,E (1983)
Log P (octanol-water):
   Value : 0.85
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 5850 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0117 atm-m3/mole
   Temp  :
   Type  : EXP
   Ref   : STAUDINGER,J & ROBERTS,PV (1996)
Atmospheric OH Rate Constant:
   Value : 0 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

WTP RISK ASSESSMENT WORK PLAN IDENTIFIED
CONSTITUENTS OF POTENTIAL CONCERN (COPC) SUPPORT DATA

Other Heavy Semivolatile Compounds (molecular weight >200 g/mole) (OSHVOL)

CHEMFATE Search Results

Return to EFDB page

CAS #: 000101-55-3 Name: 4-BROMOPHENYL PHENYL ETHER

```
*******************************************************************************
MELT     4-BROMOPHENYL PHENYL ETHER                          CAS#   101-55-3
  Melting Point  :  18.7        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1985)
*******************************************************************************

VP       4-BROMOPHENYL PHENYL ETHER                          CAS#   101-55-3
  Vapor Pressure :  0.0015      TORR
  Temperature (C):  20
  Remarks        :  EXTRAPOLATED DATA, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************

VP       4-BROMOPHENYL PHENYL ETHER                          CAS#   101-55-3
  Vapor Pressure :  1.500E-03   MM HG       EXTRAPOLATED
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979)
*******************************************************************************
```

CALLAHAN,MA ET AL. (1979)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS.; EPA-440/4-79-029A. WASHINGTON,DC: U.S.EPA.; 1979

CALLAHAN,MA ET AL. (1979A)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS-VOLUME II.; EPA-440/4-79-029 WASHINGTON,DC: U.S. EPA.; 1979A

WEAST,RC ET AL. (1985)
WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS 66TH ED; CRC PRESS; BOCA RATON, FLA; 1985

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000103-33-3
Chem Name  : AZOBENZENE
Mol Formula: C12H10N2
Mol Weight : 182.23
Melting Pt : 68 deg C
Boiling Pt : 293 deg C
Water Solubility:
   Value : 6.4 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : TAKAGISHI,T ET AL (1969)
Log P (octanol-water):
   Value : 3.82
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.000361 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : JONES,AH (1960)
pKa Dissociation Constant:
   Value : -2.95
   Temp  :
   Type  : EXP
   Ref   : HOEFNAGEL,MA ET AL. (1969)
Henry's Law Constant:
   Value : 1.35E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.55E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000107-66-4
Chem Name  : DI-N-BUTYL PHOSPHATE
Mol Formula: C8H19O4P
Mol Weight : 210.21
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 1.72E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BEILSTEIN
Log P (octanol-water):
   Value : 2.29
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 9.6E-005 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : HL X  WSOL
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 4.26E-009 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 5.27E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Hexachlorobenzene
CAS Number: 000118-74-1

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	8.0E-4	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:	1.6E+0	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	1.6E+0	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	B2		
Oral ED10:	2.6E-2	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	2.6E-2	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	1.7E+3	mg/kg	ACGIH
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:	3.3E+3	mg/L	RTECS
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	3.0E+1	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.5E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.5E+3	days	CHEMFATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.6E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.5E+3	days	CHEMFATE
Radio:		days	
Log Kow:	5.3E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.8E+2	
Density:	2.0E+0	g/mL @ 23.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.8E-5	Torr	CHEMFATE
Henry's Law:	1.3E-3	atm-m3/mol	CHEMFATE
Water Solub:	6.2E-6	mg/L	CHEMFATE
Distrib Coef:	1.1E+2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	1.8E+5		ECOTOX
Salt BCF:	5.1E+5		ECOTOX
ENVIRONMENTAL			
Fresh BCF:	9.2E+5		ECOTOX
Salt BCF:	5.1E+5		ECOTOX
Log Kow:	5.3E+0		CHEMFATE
Water Solub:	6.2E-6		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	2.3E+2	C
Boiling Point:	3.3E+2	C
Formula:	C6 Cl6	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000118-74-1 Name: HEXACHLOROBENZENE

```
*******************************************************************************
MELT    HEXACHLOROBENZENE                                    CAS#   118-74-1
  Melting Point  :  228.7       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KAO,CI & POFFENBERGER,N (1979)
*******************************************************************************

VP      HEXACHLOROBENZENE                                    CAS#   118-74-1
  Vapor Pressure :  .1089E-04   TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  LEONI,V & DARCA,SU (1976)
*******************************************************************************

VP      HEXACHLOROBENZENE                                    CAS#   118-74-1
  Vapor Pressure :  .110E-04    TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  FROM PERKOW,W. (1976)
  Abbrev. Ref.   :  KILZER,L ET AL. (1979)
*******************************************************************************

VP      HEXACHLOROBENZENE                                    CAS#   118-74-1
  Vapor Pressure :  .168E-04    TORR        CALCULATED
  Temperature (C):  25.
  Remarks        :  CALC FROM ANTOINE EQN
  Abbrev. Ref.   :  FARMER,WJ ET AL. (1980)
*******************************************************************************

VP      HEXACHLOROBENZENE                                    CAS#   118-74-1
  Vapor Pressure :  1.80E-5     MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SCHOENE,K ET AL. (1984)
*******************************************************************************
```

FARMER,WJ ET AL. (1980)
FARMER,W.J.; YANG,M.S.; LETEY,J.; SPENCER,W.F.; HEXACHLOROBENZNE: ITS VAPOR PRESSURE AND VAPOR PHASE DIFFUSION IN SOIL.; SOIL SCI. SOC. AM.; 44:676-80. 1980

KAO,CI & POFFENBERGER,N (1979)
KAO,C.I.; POFFENBERGER,N.; CHLORINATED BENZENE; IN: KIRK-OTHMER ENCYL CHEM TECH 3RD., NY,NY: WILEY INTRSCI PUBL:5:797-808; 1979

KILZER,L ET AL. (1979)

KILZER,L.; SCHEUNERT,I.; GEYER,H.; KLEIN,W.; KORTE,F.; LABORATORY SCREENING OF THE VOLATILIZATION RATES OF ORGANIC CHEMICALS FROM WATER AND SOIL.; CHEMOSPHERE.; 8:751-61.; 1979

LEONI,V & DARCA,SU (1976)
LEONI,V.; DARCA,S.U.; EXPERIMENTAL DATA AND CRITICAL REVIEW OF THE OCCURREN OF HEXACHLOROBENZENE IN THE ITALIAN ENVIRONMENT.; SCI. TOTAL ENVIRON.; 5:253-72.; 1976

SCHOENE,K ET AL. (1984)
SCHOENE,K.; BOEHMER,W.; STEINHANSES,J.; DETERMINATION OF VAPOR PRESSURES DO TO 0.01 PA BY HEADSPACE GAS-CHROMATOGRAPHY.; FRESENIUS' Z. ANAL. CHEM.; 319:903-6.; 1984

End of Search

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CHEMFATE Search Results

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CAS #: 000119-90-4 Name: 3,3'-DIMETHOXYBENZIDINE

```
*******************************************************************************
MELT    3,3'-DIMETHOXYBENZIDINE                                CAS#   119-90-4
  Melting Point  :  137-138     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      3,3'-DIMETHOXYBENZIDINE                                CAS#   119-90-4
  Vapor Pressure :  2.12E-7     MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED BY PCCHEM, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************


   MERCK INDEX (1983)
   MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH
   ED.;  WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

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CAS #: 000126-73-8 Name: TRI-N-BUTYL PHOSPHATE

```
*****************************************************************************
MELT    TRI-N-BUTYL PHOSPHATE                                CAS#   126-73-8
  Melting Point  :  -79          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*****************************************************************************

VP      TRI-N-BUTYL PHOSPHATE                                CAS#   126-73-8
  Vapor Pressure :  1.20E-04     MM HG       CALC
  Temperature (C):  25
  Remarks        :
             1   :  SRC RECOMMENDED VALUE
             2   :   EXTRAPOLATED FROM TEMP RANGE 114 DEG C(0.8 MMHG) - 160-16
                 DEG C(15 MMHG)
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************
```

ALDRICH (1988)
ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI:
ALDRICH CHEM CO.; 1988

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI
AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY
WILEY-INTERSCIENCE. 2:PP.1325; 1986

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000128-37-0
Chem Name  : 2,6-DI-T-BUTYL-4-METHYLPHENOL (BHT)
Mol Formula: C15H24O
Mol Weight : 220.36
Melting Pt : 71 deg C
Boiling Pt : 265 deg C
Water Solubility:
   Value : 0.6 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : INUI,H ET AL. (1979A)
Log P (octanol-water):
   Value : 5.10
   Type  : EXP
   Ref   : TSCATS
Vapor Pressure:
   Value : 0.00516 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : PERRY,RH & GREEN,D (1984)
pKa Dissociation Constant:
   Value : 12.2
   Temp  :
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 4.12E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.83E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000131-89-5
Chem Name  : 2-CYCLOHEXYL-4,6-DINITROPHENOL
Mol Formula: C12H14N2O5
Mol Weight : 266.26
Melting Pt : 107 deg C
Boiling Pt :
Water Solubility:
   Value : 15 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 4.12
   Type  : EXP
   Ref   : ELLINGTON,JT & STANCIL,FE (1988)
Vapor Pressure:
   Value : 4.19E-008 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value : 4.52
   Temp  : 25 deg C
   Type  : EST
   Ref   : LIPNICK,RL ET AL. (1986)
Henry's Law Constant:
   Value : 5.54E-008 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.02E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CAS #: 000133-06-2 Name: CAPTAN

```
*****************************************************************************
MELT     CAPTAN                                                CAS#   133-06-2
  Melting Point  :  178          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WORTHING,CR & WALKER,SB (1983)
*****************************************************************************

VP       CAPTAN                                                CAS#   133-06-2
  Vapor Pressure :  .1E-04       TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UPPER LIM
  Abbrev. Ref.   :  MARTIN,H & WORTHING,CR (1977)
*****************************************************************************

VP       CAPTAN                                                CAS#   133-06-2
  Vapor Pressure :  6.0E-5       MM HG
  Temperature (C):  25.25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  GILE,JD & GILLETT,JW (1979)
*****************************************************************************
```

GILE,JD & GILLETT,JW (1979)
GILE,J.D.; GILLETT,J.W.; FATE OF SELECTED FUNGICIDES IN A TERRESTRIAL LABORATORY ECOSYSTEM.; J. AGRIC. FOOD CHEM.; 27:1159-64.; 1979

MARTIN,H & WORTHING,CR (1977)
MARTIN,H.; WORTHING,C.R.; PESTICIDE MANUAL. FIFTH EDITION, BRITISH CROP PROTECTION COUNCIL. 563 PP.; 1977

WORTHING,CR & WALKER,SB (1983)
WORTHING,C.R.; WALKER,S.B.; PESTICIDE MANUAL 7TH ED; BRITISH CROP PROTECTIO COUNCIL. LAVENHAM SUFFOLK, ENGLAND: LAVENHAM PRESS LTD; 1983

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Data From SRC PhysProp Database:

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References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 023950-58-5
Chem Name  : PRONAMIDE
Mol Formula: C12H11Cl2NO
Mol Weight : 256.13
Melting Pt : 155 deg C
Boiling Pt :
Water Solubility:
   Value : 15 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 3.43
   Type  : EXP
   Ref   : ELLINGTON,JT & STANCIL,FE (1988)
Vapor Pressure:
   Value : 4.35E-007 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : TOMLIN,C (1994)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.77E-009 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.32E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 026140-60-3
Chem Name  : TERPHENYL
Mol Formula: C18H14
Mol Weight : 230.31
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 0.215 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 5.52
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 3.09E-006 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.18E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 9.19E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CAS #: 000510-15-6 Name: CHLOROBENZILATE

```
*******************************************************************************
MELT     CHLOROBENZILATE                                        CAS#   510-15-6
  Melting Point   :  35-37        DEGC
  Remarks         :  SRC RECOMMENDED VALUE
  Abbrev. Ref.    :  MARTIN,H & WORTHING,CR (1977)
*******************************************************************************

VP       CHLOROBENZILATE                                        CAS#   510-15-6
  Vapor Pressure  :  2.2E-6       MM HG
  Temperature (C) :  20
  Remarks         :  SRC RECOMMENDED VALUE
  Abbrev. Ref.    :  MARTIN,H & WORTHING,CR (1977)
*******************************************************************************
```

MARTIN,H & WORTHING,CR (1977)
MARTIN,H.; WORTHING,C.R.; PESTICIDE MANUAL. FIFTH EDITION, BRITISH CROP PROTECTION COUNCIL. 563 PP.; 1977

End of Search

CHEMFATE Search Results

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CAS #: 000057-24-9 Name: STRYCHNIDIN-10-ONE

```
*****************************************************************************
MELT    STRYCHNIDIN-10-ONE                                  CAS#    57-24-9
  Melting Point  :  268-290     DEGC
  Remarks        :  DEPENDS ON SPEED OF HEATING, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP      STRYCHNIDIN-10-ONE                                  CAS#    57-24-9
  Vapor Pressure :  9.43E-12    MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************


   MERCK INDEX (1983)
   MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH
   ED.;  WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

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CAS #: 000060-11-7 Name: 4-(DIMETHLAMINO)AZOBENZENE

```
*****************************************************************************
MELT     4-(DIMETHLAMINO)AZOBENZENE                          CAS#     60-11-7
  Melting Point  :  114-117      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP       4-(DIMETHLAMINO)AZOBENZENE                          CAS#     60-11-7
  Vapor Pressure :  7E-8         MM HG
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM DATA RANGE 356-407 DEG K, SRC RECOMMENDE
                    VALUE
  Abbrev. Ref.   :  CAMPANELLI,AR ET AL. (1985)
*****************************************************************************
```

CAMPANELLI,AR ET AL. (1985)
CAMPANELLI,A.R.; FERRO,D.; PAVEL,N.V.; STUDY OF THE 4:1 INCLUSION COMPOUND BETWEEN DEOXYCHOLIC ACID AND (E)-P-DIMETHYLAMINOAZOBENZENE BY VAPOR PRESSUR MEASUREMENTS.; THERMOCHIM. ACTA; 87:231-8; 1985

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

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References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000603-34-9
Chem Name  : TRIPHENYLAMINE
Mol Formula: C18H15N
Mol Weight : 245.33
Melting Pt : 127 deg C
Boiling Pt : 365 deg C
Water Solubility:
   Value : 0.315 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 5.74
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.000392 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : FORWARD,MV ET AL. (1949)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 5.41E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 2E-010 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

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CAS #: 000608-93-5 Name: PENTACHLOROBENZENE

```
*****************************************************************************
MELT     PENTACHLOROBENZENE                                  CAS#   608-93-5
  Melting Point  :  86          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEAST,RC ET AL. (1985)
*****************************************************************************

VP       PENTACHLOROBENZENE                                  CAS#   608-93-5
  Vapor Pressure :  2.19E-3     MM HG
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM A LIQUID STATE FROM A T-RANGE OF
                    98.6-276.0 DEG C WITH FUGACITY RATIO CORRECTION,
                    EXPERIMENTAL DATA FROM PERRY,RH & GREEN (1984), SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  MACKAY,D & SHIU,WY (1981)
*****************************************************************************
```

MACKAY,D & SHIU,WY (1981)
MACKAY,D.; SHIU,W.Y.; A CRITICAL REVIEW OF HENRY'S LAW CONSTANTS FOR CHEMICALS OF ENVIRONMENTAL INTEREST.; J. PHYS. CHEM. REF. DATA.; 19:1175-99 1981

WEAST,RC ET AL. (1985)
WEAST,R.C.; ASTLE,M.J.; BEYER,W.H.; CRC HANDBOOK OF CHEMISTRY AND PHYSICS 66TH ED; CRC PRESS; BOCA RATON, FLA; 1985

End of Search

CHEMFATE Search Results

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CAS #: 000067-72-1 Name: HEXACHLOROETHANE

```
*****************************************************************************
MELT    HEXACHLOROETHANE                                        CAS#    67-72-1
  Melting Point  :  186.8        DEGC
  Remarks        :  SUBLIMES, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP      HEXACHLOROETHANE                                        CAS#    67-72-1
  Vapor Pressure :  0.21         MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ARCHER,WL (1979)
*****************************************************************************
```

ARCHER,WL (1979)
ARCHER,W.L.; OTHER CHLOROETHANES.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 5:722-42.; 1979

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

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CAS #: 000070-30-4 Name: HEXACHLOROPHENE

```
*******************************************************************************
MELT    HEXACHLOROPHENE                                          CAS#    70-30-4
  Melting Point  :  164-165     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      HEXACHLOROPHENE                                          CAS#    70-30-4
  Vapor Pressure :  1.5E-10     MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATION BASED ON MEASURED WATER SOLUBILITY AND ESTIMATE
                    HENRY'S LAW CONSTANT, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

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CHEMFATE Search Results

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CAS #: 000077-47-4 Name: HEXACHLOROCYCLOPENTADIENE

```
*******************************************************************************
MELT    HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Melting Point  :  11.34       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  STEVENS,JE (1979)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  .6300E-01   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  BELL,MA ET AL. (1978)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  .81E-01     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  FROM VERSCHUEREN,K. (1977)
  Abbrev. Ref.   :  KILZER,L ET AL. (1979)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  .8E-01      TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  WOLFE,NL ET AL. (1982)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  0.10        MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  ATALLAH,YH ET AL. (1980)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  6.000E-02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************

VP      HEXACHLOROCYCLOPENTADIENE                          CAS#    77-47-4
  Vapor Pressure :  5.96E-2     MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

ATALLAH,YH ET AL. (1980)
ATALLAH,Y.H.; WHITACRE,D.M.; BUTZ,R.G.; FATE OF HEXACHLOROCYCLOPENTADIENE I THE ENVIRONMENT.; PRESENTED BEFORE THE DIV. OF ENVIRON. CHEM., AMERICAN CHEMICAL SOCIETY, AUGUST 24-29, 1980. SAN FRANCISCO, CA.; 1980

BELL,MA ET AL. (1978)
BELL,M.A.; EWING,R.A.; LUTZ,G.A.; REVIEWS OF THE ENVIRONMENTAL EFFECTS OF POLLUTANTS: XII. HEXACHLOROCYCLOPENTADIENE.; EPA-600/1-78-047. COLUMBUS, O U.S. EPA. PP.94.; 1978

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

KILZER,L ET AL. (1979)
KILZER,L.; SCHEUNERT,I.; GEYER,H.; KLEIN,W.; KORTE,F.; LABORATORY SCREENING OF THE VOLATILIZATION RATES OF ORGANIC CHEMICALS FROM WATER AND SOIL.; CHEMOSPHERE.; 8:751-61.; 1979

STEVENS,JE (1979)
STEVENS,J.E.; CHLORINATED DERIVATIVES OF CYCLOPENTADIENES; IN: KIRK-OTHMER ENCYCL CHEM TECH 3RD ED NY,NY: WILEY 5:791-7; 1979

WOLFE,NL ET AL. (1982)
WOLFE,N.L.; ZEPP,R.G.; SCHLOTZHAUER,P.; SINK,M.; TRANSFORMATION PATHWAYS OF HEXACHLOROCYCLOPENTADIENE IN THE AQUATIC ENVIRONMENT.; CHEMOSPHERE.; 11:91-101.; 1982

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000822-06-0 Name: 1,6-DIISOCYANATOHEXANE

```
*****************************************************************************
VP      1,6-DIISOCYANATOHEXANE                              CAS#   822-06-0
  Vapor Pressure :  0.03        MM HG       EST
  Temperature (C):  25
  Abbrev. Ref.   :  GOLDBERG,NA & KUCHERYAVYI,VI (1960)
*****************************************************************************
```

GOLDBERG,NA & KUCHERYAVYI,VI (1960)
GOLDBERG,N.A.; KUCHERYAVYI,V.I.; SOME PHYSICOCHEMICAL PROPERTIES OF HEXAMETHYLENE DIISOCYNATE.; PRIKLAD. KHIM.; 33:1912-13.; 1960

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000822-06-0
Chem Name  : HEXAMETHYLENE DIISOCYANATE
Mol Formula: C8H12N2O2
Mol Weight : 168.20
Melting Pt : -67 deg C
Boiling Pt : 255 deg C
Water Solubility:
   Value : 117 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 3.20
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 0.03 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : GOLDBERG,NA & KUCHERYAVYI,VI (1960)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 4.8E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 7.74E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : ATKINSON,R (1988)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000082-68-8 Name: PENTACHLORONITROBENZENE

```
*****************************************************************************
VP      PENTACHLORONITROBENZENE                              CAS#    82-68-8
  Vapor Pressure :  .5E-04      .113E-03    .113E-03    TORR        MEASURED
  Temperature (C):  20.25       25.00       25.25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  GILE,JD & GILLETT,JW (1979)
*****************************************************************************
```

GILE,JD & GILLETT,JW (1979)
GILE,J.D.; GILLETT,J.W.; FATE OF SELECTED FUNGICIDES IN A TERRESTRIAL LABORATORY ECOSYSTEM.; J. AGRIC. FOOD CHEM.; 27:1159-64.; 1979

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000082-68-8
Chem Name  : PENTACHLORONITROBENZENE
Mol Formula: C6Cl5NO2
Mol Weight : 295.34
Melting Pt : 144 deg C
Boiling Pt : 328 deg C
Water Solubility:
   Value : 0.44 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 4.64
   Type  : EXP
   Ref   : SANGSTER (1994)
Vapor Pressure:
   Value : 5E-005 mm Hg
   Temp  : 20 deg C
   Type  : EXP
   Ref   : GILE,JD & GILLETT,JW (1979)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 4.42E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 7.23E-015 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000082-68-8 Name: PENTACHLORONITROBENZENE

```
*****************************************************************************
VP      PENTACHLORONITROBENZENE                              CAS#    82-68-8
  Vapor Pressure :  .5E-04      .113E-03    .113E-03    TORR        MEASURED
  Temperature (C):  20.25       25.00       25.25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  GILE,JD & GILLETT,JW (1979)
*****************************************************************************
```

GILE,JD & GILLETT,JW (1979)
GILE,J.D.; GILLETT,J.W.; FATE OF SELECTED FUNGICIDES IN A TERRESTRIAL LABORATORY ECOSYSTEM.; J. AGRIC. FOOD CHEM.; 27:1159-64.; 1979

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Hexachlorobutadiene
CAS Number: 000087-68-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	2.0E-4	mg/kg/day	HEAST
Inhal RfD:		mg/kg/day	
Oral Slope:	7.8E-2	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	C		
Inhal Slope:	7.7E-2	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	C		
Oral ED10:	1.7E+0	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	C		
Inhal ED10:	1.7E+0	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	C		
Oral LD50:	4.6E+1	mg/kg	ACGIH
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	6.0E+1	µg/L	ECOTOX
Salt Ecol LC50:	4.5E+2	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.4E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.5E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	4.8E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.6E+2	
Density:	1.6E+0	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.2E-1	Torr	CHEMFATE
Henry's Law:	8.1E-3	atm-m3/mol	CHEMFATE
Water Solub:	3.2E+0	mg/L	CHEMFATE
Distrib Coef:	7.6E+3	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	6.0E+1		VER_BCF
Salt BCF:	1.0E+4		ECOTOX
ENVIRONMENTAL			
Fresh BCF:	2.3E+3		VER_BCF
Salt BCF:	1.0E+4		ECOTOX
Log Kow:	4.8E+0		CHEMFATE
Water Solub:	3.2E+0		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-2.1E+1	C
Boiling Point:	2.2E+2	C
Formula:	C4 Cl6	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000087-68-3 Name: HEXACHLOROBUTADIENE

```
*******************************************************************************
VP      HEXACHLOROBUTADIENE                                  CAS#    87-68-3
  Vapor Pressure :  0.076       MM HG       CALC
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM EXPERIMENTAL DATA BEGINNING AT 70 DEG C
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************

VP      HEXACHLOROBUTADIENE                                  CAS#    87-68-3
  Vapor Pressure :  2.213E-01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Pentachlorophenol (PCP)
CAS Number: 000087-86-5

TOXICITY

Parameter	Value		Unit	Source
Oral RfD:	3.0E-2		mg/kg/day	IRIS
Inhal RfD:			mg/kg/day	
Oral Slope:	1.2E-1		(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2			
Inhal Slope:			(mg/kg/day)^-1	
Inhal Wt-of-Evid:				
Oral ED10:			mg/kg/day	
Oral ED10 Wgt:				
Inhal ED10:			mg/kg/day	
Inhal ED10 Wgt:				
Oral LD50:	1.5E+2		mg/kg	ACGIH
Dermal LD50:	9.6E+1		mg/kg	ACGIH
Gas Inhal LC50:			ppm	
Dust Inhal LC50:			mg/L	
ACUTE				
Fresh CMC:	1.9E+1	F, K bb	µg/L	WATCRIT
Salt CMC:	1.3E+1		µg/L	WATCRIT
CHRONIC				
Fresh CCC:	1.5E+1	F, K bb	µg/L	WATCRIT
Salt CCC:	7.9E+0		µg/L	WATCRIT
Fresh Ecol LC50:	4.0E-1		µg/L	ECOTOX
Salt Ecol LC50:	3.7E+1		µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:		days	
Photolysis:	4.2E+0	days	CHEMFATE
Biodeg:	4.8E+1	days	CHEMFATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:		days	
Photolysis:	4.2E+0	days	CHEMFATE
Biodeg:	4.8E+1	days	CHEMFATE
Radio:		days	
Log Kow:	5.1E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.7E+2	
Density:	2.0E+0	g/mL @ 22.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	3.2E-5	Torr	CHEMFATE
Henry's Law:	2.4E-8	atm-m3/mol	CHEMFATE
Water Solub:	2.0E+3	mg/L	CHEMFATE
Distrib Coef:	1.2E+0	ml/g	RTI_ION
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	4.5E+4		ECOTOX
Salt BCF:	1.3E+3		ECOTOX
ENVIRONMENTAL			
Fresh BCF:	4.5E+4		ECOTOX
Salt BCF:	3.8E+3		ECOTOX
Log Kow:	5.1E+0		CHEMFATE
Water Solub:	2.0E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	1.7E+2	C
Boiling Point:		C
Formula:	C6 H Cl5 O	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000087-86-5 Name: PENTACHLOROPHENOL

```
*****************************************************************************
VP      PENTACHLOROPHENOL                                    CAS#    87-86-5
  Vapor Pressure :  1.1E-4      MM HG       MEAS
  Temperature (C):  20
  Abbrev. Ref.   :  SCOW,K ET AL. (1980)
*****************************************************************************

VP      PENTACHLOROPHENOL                                    CAS#    87-86-5
  Vapor Pressure :  3.17E-5     MM HG       CALC
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM DATA FOR THE LIQUID MATERIAL OBTAINED IN
                    THE RANGE 192.2-309.3 DEG C AND CONVERTED TO VAPOR PRESSUR
                    FOR THE SOLID. SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

SCOW,K ET AL. (1980)
SCOW,K.; GOYER,M.; PAYNE,E.; PERWACK,J.; THOMAS,R.; WALLACE, . ; WALKER,P.; WOOD,M.; AN EXPOSURE AND RISK ASSESSMENT FOR PENTACHLOROPHENOL.; EPA-440/4-81-021. (NTIS PB85-211944). CAMBRIDGE,MA: ARTHUR D. LITTLE INC. PP.195.; 1980

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000091-94-1 Name: 3,3'-DICHLOROBENZIDINE

```
*******************************************************************************
MELT    3,3'-DICHLOROBENZIDINE                                  CAS#    91-94-1
  Melting Point  :  131-132     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SIKKA,HC ET AL. (1978)
*******************************************************************************

VP      3,3'-DICHLOROBENZIDINE                                  CAS#    91-94-1
  Vapor Pressure :  3.71E-8     MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED USING PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************
```

SIKKA,HC ET AL. (1978)
SIKKA,H.C.; APPLETON,H.T.; BANERJEE,S.; FATE OF 3,3'-DICHLOROBENZIDINE IN AQUATIC ENVIRONMENTS.; EPA-600/3-78-068. SYRACUSE,NY: SYRACUSE RES. CORP.; 1978

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Tetrachlorobenzene, 1,2,4,5-
CAS Number: 000095-94-3

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	3.0E-4	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	8.9E+1	µg/L	ECOTOX
Salt Ecol LC50:	1.2E+2	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.2E+3	days	CHEMFATE
Volatility:	1.3E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.2E+3	days	CHEMFATE
Volatility:	1.4E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	4.8E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.2E+2	
Density:	1.9E+0	g/mL @ 22.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	5.4E-3	Torr	CHEMFATE
Henry's Law:	2.6E-3	atm-m3/mol	CHEMFATE
Water Solub:	5.9E-1	mg/L	CHEMFATE
Distrib Coef:	1.1E+1	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	4.1E+3		ECOTOX
Salt BCF:			
Log Kow:	4.8E+0		CHEMFATE
Water Solub:	5.9E-1		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	1.4E+2	C
Boiling Point:	2.4E+2	C
Formula:	C6 H2 Cl4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000095-94-3 Name: 1,2,4,5-TETRACHLOROBENZENE

```
*****************************************************************************
MELT    1,2,4,5-TETRACHLOROBENZENE                          CAS#    95-94-3
  Melting Point  :  139.5       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KAO,CI & POFFENBERGER,N (1979)
*****************************************************************************

VP      1,2,4,5-TETRACHLOROBENZENE                          CAS#    95-94-3
  Vapor Pressure :  0.0054      MM HG       CALC
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE, EXTRAPOLATED FROM HIGHER EXPERIMENT
                    TEMPERATURES (146-245 DEG C) AND CORRECTED FOR A VAPOR
                    PRESSURE FOR A SOLID USING A FUGACITY CORRECTION FACTOR
  Abbrev. Ref.   :  MACKAY,D ET AL. (1982)
*****************************************************************************
```

KAO,CI & POFFENBERGER,N (1979)
KAO,C.I.; POFFENBERGER,N.; CHLORINATED BENZENE; IN: KIRK-OTHMER ENCYL CHEM TECH 3RD., NY,NY: WILEY INTRSCI PUBL:5:797-808; 1979

MACKAY,D ET AL. (1982)
MACKAY,D.; BOBRA,A.; CHAN,D.W.; SHIU,W.Y.; VAPOR PRESSURE CORRELATIONS FOR LOW-VOLATILITY ENVIRONMENTAL CHEMICALS.; ENVIRON. SCI. TECHNOL.; 16:645-9.; 1982

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value. References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000096-69-5
Chem Name  : 4,4'-Thiobis(6-tert-butyl-3-cresol)
Mol Formula: C22H30O2S
Mol Weight : 358.55
Melting Pt : 162 deg C
Boiling Pt :
Water Solubility:
   Value : 0.00191 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 8.24
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 8.59E-011 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 2.76E-012 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.3E-010 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WN & HOWARD,PH (1993)
```

Back To PhysProp Demo Page

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Trinitrobenzene, 1,3,5-
CAS Number: 000099-35-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	3.0E-2	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	2.8E+2	mg/kg	RTECS
Dermal LD50:	2.0E+3	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	3.4E+2	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:		days	
Photolysis:		days	
Biodeg:		days	
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:		days	
Photolysis:		days	
Biodeg:		days	
Radio:		days	
Log Kow:	1.2E+0		PHYSPROP

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.1E+2	
Density:	1.5E+0	g/mL @ 152.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	6.4E-6	Torr	PHYSPROP
Henry's Law:	3.3E-10	atm-m3/mol	PHYSPROP
Water Solub:	2.8E+2	mg/L	PHYSPROP
Distrib Coef:	2.2E+0	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	1.2E+0		PHYSPROP
Water Solub:	2.8E+2		PHYSPROP
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	1.2E+2	C
Boiling Point:	3.2E+2	C
Formula:	C6 H3 N3 O6	

CLASS INFORMATION

Class	Parent Substance

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000099-35-4
Chem Name  : 1,3,5-TRINITROBENZENE
Mol Formula: C6H3N3O6
Mol Weight : 213.11
Melting Pt : 121.5 deg C
Boiling Pt : 315 deg C
Water Solubility:
   Value : 278 mg/L
   Temp  : 15 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.18
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 6.44E-006 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : OHE,S (1976)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.31E-010 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.3E-015 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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WTP RISK ASSESSMENT WORK PLAN IDENTIFIED
CONSTITUENTS OF POTENTIAL CONCERN (COPC) SUPPORT DATA

Other Light Semivolatile Compounds (molecular weight >200 g/mole) (OLSVOL)

CHEMFATE Search Results

Return to EFDB page

CAS #: 000100-21-0 Name: TEREPHTHALIC ACID

```
*****************************************************************************
MELT    TEREPHTHALIC ACID                                    CAS#   100-21-0
  Melting Point  :  >300        DEGC
  Remarks        :  WITH SUBLIMATION OCCURRING BEFORE MELTING, SRC RECOMMENDED
                    VALUE
  Abbrev. Ref.   :  BEMIS,AG ET AL. (1982)
*****************************************************************************

VP      TEREPHTHALIC ACID                                    CAS#   100-21-0
  Vapor Pressure :  9.2E-6      MM HG
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM 120 DEG C USING DATA FROM TOWLE ET AL
                    1968, SRC SUGGESTED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************
```

BEMIS,AG ET AL. (1982)
BEMIS,A.G.; DINDORF,J.A.; HORWOOD,B.; SAMANS,C.; PHTHALIC ACIDS, AND OTHER BENZENEPOLYCARBOXYLIC ACIDS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 17:732-77.; 1982

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000101-77-9 Name: 4,4'METHYLENEDIANILINE

```
*******************************************************************************
MELT    4,4'METHYLENEDIANILINE                                  CAS#   101-77-9
  Melting Point  :  89.0        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MOORE,WM (1978)
*******************************************************************************

VP      4,4'METHYLENEDIANILINE                                  CAS#   101-77-9
  Vapor Pressure :  .10E 02     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UPPER LIM
  Abbrev. Ref.   :  DORIGAN,J ET AL. (1976)
*******************************************************************************

VP      4,4'METHYLENEDIANILINE                                  CAS#   101-77-9
  Vapor Pressure :  2.97        MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED VIA CLAUSIUS CLAPEYRON EQN USING A MEASURED VP O
                    7.5 MM HG AT 229 DEG C BOUBLIK ET AL 1984, SRC RECOMMENDED
                    VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************
```

DORIGAN,J ET AL. (1976)
DORIGAN,J.; FULLER,B.; DUFFY,R.; PRELIMINARY SCORING OF SELECTED ORGANIC AI POLLUTANTS. APPENDIX III-CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS F THROUGH N.; EPA-450/3-77-008D. RESEARCH TRIANGLE PARK,NC: U.S. EPA. PP.303 1976

MOORE,WM (1978)
MOORE,W.M.; METHYLENEDIANILINE; IN: KIRK-OTHMER ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY. 3RD ED. NEW YORK: WILEY & SONS 2:338-48; 1978

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000101-84-8 Name: DIPHENYL ETHER

```
*****************************************************************************
MELT    DIPHENYL ETHER                                        CAS#   101-84-8
  Melting Point  :  28          DEG C
  Remarks        :
             1   :  HIGH PRODUCTION VOLUME SUBMISSION DATA
             2   :   HPV: DIPHENYL OXIDE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************

VP      DIPHENYL ETHER                                        CAS#   101-84-8
  Vapor Pressure :  0.02        MM HG       MEASURED
  Temperature (C):  20
  Remarks        :
             1   :  HIGH PRODUCTION VOLUME SUBMISSION DATA
             2   :   HPV: DIPHENYL OXIDE
  Abbrev. Ref.   :  US EPA (2004)
*****************************************************************************
```

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-51-4 Name: 1,4-BENZOQUINONE

```
*******************************************************************************
MELT    1,4-BENZOQUINONE                                        CAS#   106-51-4
  Melting Point  :  115.7        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      1,4-BENZOQUINONE                                        CAS#   106-51-4
  Vapor Pressure :  37.5         MM HG
  Temperature (C):  20
  Remarks        :  EXTRAPOLATED VALUE, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEBER,RC ET AL. (1981)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

WEBER,RC ET AL. (1981)
WEBER,R.C.; PARKER,P.A.; BOWSER,M.; VAPOR PRESSURE DISTRIBUTION OF SELECTED ORGANIC CHEMICALS.; EPA-600/2-81-021. CINCINNATI,OH: U.S.EPA. PP.39.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-89-8 Name: EPICHLOROHYDRIN

```
*****************************************************************************
MELT    EPICHLOROHYDRIN                                        CAS#   106-89-8
  Melting Point  :  -57.2       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIESSER,GH (1979)
*****************************************************************************

VP      EPICHLOROHYDRIN                                        CAS#   106-89-8
  Vapor Pressure :  .1813E 02   TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1967)
*****************************************************************************

VP      EPICHLOROHYDRIN                                        CAS#   106-89-8
  Vapor Pressure :  16.44       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

GALLANT,RW (1967)
GALLANT,R.W.; PHYSICAL PROPERTIES OF HYDROCARBONS. XII. C2-C4 OXIDES.; HYDROCARBON PROCESS.; 46:143-150.; 1967

RIESSER,GH (1979)
RIESSER,G.H.; CHLOROHYDRINS.; KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. NY,N WILEY-INTERSCIENCE. 5:858.; 1979

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Dibromoethane, 1,2-
CAS Number: 000106-93-4

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:	5.7E-5	mg/kg/day	HEAST
Oral Slope:	8.5E+1	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	7.7E-1	(mg/kg/day)^-1	IRIS
Inhal Wt-of-Evid:	B2		
Oral ED10:	2.6E-3	mg/kg/day	SPHEM
Oral ED10 Wgt:	B2		
Inhal ED10:	2.6E-3	mg/kg/day	SPHEM
Inhal ED10 Wgt:	B2		
Oral LD50:	1.2E+2	mg/kg	ACGIH
Dermal LD50:	3.0E+2	mg/kg	RTECS
Gas Inhal LC50:	4.0E+2	ppm	RTECS
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.5E+4	µg/L	ECOTOX
Salt Ecol LC50:	4.8E+3	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	2.9E+3	days	CHEMFATE
Volatility:	1.2E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	2.9E+3	days	CHEMFATE
Volatility:	1.3E+0	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.0E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	No	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.9E+2	
Density:	2.2E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.3E+1	Torr	CHEMFATE
Henry's Law:	7.4E-4	atm-m3/mol	CHEMFATE
Water Solub:	4.0E+3	mg/L	CHEMFATE
Distrib Coef:	8.5E-2	ml/g	SSG_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.0E+0		CHEMFATE
Water Solub:	4.0E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	9.9E+0	C
Boiling Point:	1.3E+2	C
Formula:	C2 H4 Br2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000106-93-4 Name: ETHANE, 1,2-DIBROMO-

```
*******************************************************************************
MELT    ETHANE, 1,2-DIBROMO-                                  CAS#   106-93-4
  Melting Point  :  9.79        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

MELT    ETHANE, 1,2-DIBROMO-                                  CAS#   106-93-4
  Melting Point  :  9.8         DEG C
  Remarks        :
            1    :  IARC V15: 195
            2    :   HPV: ETHANE, 1,2-DIBROMO
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************

VP      ETHANE, 1,2-DIBROMO-                                  CAS#   106-93-4
  Vapor Pressure :  .8300E+01   .1420E+02   .3000E+02   TORR        MEASURED
  Temperature (C):  15.0        25.0        40.0
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  GALLANT,RW (1968)
*******************************************************************************

VP      ETHANE, 1,2-DIBROMO-                                  CAS#   106-93-4
  Vapor Pressure :  11.2        MM HG       MEAS
  Temperature (C):  25
  Abbrev. Ref.   :  CALL,F (1957)
*******************************************************************************

VP      ETHANE, 1,2-DIBROMO-                                  CAS#   106-93-4
  Vapor Pressure :  13.3        MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

CALL,F (1957)
CALL,F.; DETERMINATION OF THE VAPOUR PRESSURE OF ETHYLENE DIBROMIDE.; J. SC FOOD. AGRIC.; 8:81-5.; 1957

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

GALLANT,RW (1968)
GALLANT,R.W.; PHYSICAL PROPERTIES OF HYDROCARBONS. PART XXIII. BROMINATED HYDROCARBONS.; HYDROCARBON PROCESS.; 47:128-36.; 1968

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000107-21-1 Name: ETHYLENE GLYCOL

```
*****************************************************************************
MELT    ETHYLENE GLYCOL                                        CAS#   107-21-1
  Melting Point  :  -12.6       DEGC
  Remarks        :  THE FREEZING IS IN DOUBT BECAUSE OF THE TENDENCY TO
                    SUPERCOOL AND FORM A GLASS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP      ETHYLENE GLYCOL                                        CAS#   107-21-1
  Vapor Pressure :  .12E 00     TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  FAY,RH (1978)
*****************************************************************************

VP      ETHYLENE GLYCOL                                        CAS#   107-21-1
  Vapor Pressure :  0.092       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

FAY,RH (1978)
FAY,R.H.; ANTIFREEZES AND DEICING FLUIDS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 3:79-95.; 1978

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-60-1 Name: BIS(1-CHLOROISOPROPYL) ETHER

```
*******************************************************************************
MELT    BIS(1-CHLOROISOPROPYL) ETHER                        CAS#   108-60-1
  Melting Point  :  -97          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************

VP      BIS(1-CHLOROISOPROPYL) ETHER                        CAS#   108-60-1
  Vapor Pressure :  .78E 00      TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  AV OF RANGE .71-.85 TORR
  Abbrev. Ref.   :  KIRWIN,CJJR & SANDMEYER,EE (1981)
*******************************************************************************

VP      BIS(1-CHLOROISOPROPYL) ETHER                        CAS#   108-60-1
  Vapor Pressure :  0.85         MM HG
  Temperature (C):  20
  Remarks        :
            1    :  REPORTED VALUE
            2    :   NOT KNOWN IF EXPERIMENTALLY DETERMINED
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************

VP      BIS(1-CHLOROISOPROPYL) ETHER                        CAS#   108-60-1
  Vapor Pressure :  0.88         MM HG
  Temperature (C):  25
  Remarks        :  INTERPRETATED FROM EXPERIMENTAL DATA OVER THE TEMPERATURE
                    RANGE OF 20-97 DEG C. SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KAWAMOTO,K & URANO,K (1989)
*******************************************************************************
```

CALLAHAN,MA ET AL. (1979A)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS-VOLUME II.; EPA-440/4-79-029 WASHINGTON,DC: U.S. EPA.; 1979A

KAWAMOTO,K & URANO,K (1989)
KAWAMOTO,K.;URANO,K.; PARAMETERS FOR PREDICTING FATE OF ORGANOCHLORINE PESTICIDES IN THE ENVIRONMENT. (I) OCTANOL-WATER AND AIR-WATER PARTITION COEFFICIENTS.; CHEMOSPHERE; 18:1987-96; 1989

KIRWIN,CJJR & SANDMEYER,EE (1981)
KIRWIN,C.J. JR.; SANDMEYER,E.E.; ETHERS.; IN: PATTY'S INDUSTRIAL HYGIENE AN

TOXICOLOGY. 3RD REV. ED.; 2A:2491-565.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000108-93-0 Name: CYCLOHEXANOL

```
*******************************************************************************
MELT     CYCLOHEXANOL                                          CAS#   108-93-0
  Melting Point  :  24          DEG C
  Remarks        :
            1    :  BASF/AG (1993)
            2    :   HPV: CYCLOHEXANOL
  Abbrev. Ref.   :  US EPA (2004)
*******************************************************************************

VP       CYCLOHEXANOL                                          CAS#   108-93-0
  Vapor Pressure :  .1125E 01   TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  FISHER,WB & VANPEPPEN,JF (1978)
*******************************************************************************

VP       CYCLOHEXANOL                                          CAS#   108-93-0
  Vapor Pressure :  8.000E-01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

FISHER,WB & VANPEPPEN,JF (1978)
FISHER,W.B.; VANPEPPEN,J.F.; CYCLOHEXANOL AND CYCLOHEXANONE.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 7:410-6.; 1978

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC: USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000109-77-3
Chem Name  : MALONONITRILE
Mol Formula: C3H2N2
Mol Weight : 66.06
Melting Pt : 32 deg C
Boiling Pt : 218.5 deg C
Water Solubility:
   Value : 1.33E+005 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KIRK-OTHMER ENCYCL 4th ed 15:941 (1995)
Log P (octanol-water):
   Value : -0.60
   Type  : EXP
   Ref   : TANII,H & HASHIMOTO,K (1985)
Vapor Pressure:
   Value : 0.2 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : 11.4
   Temp  :
   Type  : EXP
   Ref   : KIRK-OTHMER ENCYCL 4th ed 15:941 (1995)
Henry's Law Constant:
   Value : 1.31E-007 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.37E-014 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

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CAS #: 000109-99-9 Name: TETRAHYDROFURAN

```
*****************************************************************************
VP      TETRAHYDROFURAN                                      CAS#   109-99-9
  Vapor Pressure :  .8400E+02   .1320E+03   .1980E+03   TORR        MEASURED
  Temperature (C):  0.0         20.0        30.0
  Abbrev. Ref.   :  VERSCHUEREN,K (1977)
*****************************************************************************

VP      TETRAHYDROFURAN                                      CAS#   109-99-9
  Vapor Pressure :  1.622E+02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

VERSCHUEREN,K (1977)
VERSCHUEREN,K.; HANDBOOK OF ENVIRONMENTAL DATA ON ORGANIC CHEMICALS.; NEW YORK, NY: VAN NOSTRAND REINHOLD COMPANY.; 1977

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000109-99-9
Chem Name  : TETRAHYDROFURAN
Mol Formula: C4H8O
Mol Weight : 72.11
Melting Pt : -108.3 deg C
Boiling Pt : 65 deg C
Water Solubility:
   Value : 1E+006 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : DUNLOP,AP (1966)
Log P (octanol-water):
   Value : 0.46
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 162 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value : -2.08
   Temp  :
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Henry's Law Constant:
   Value : 7.05E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : CABANI,S ET AL. (1971A)
Atmospheric OH Rate Constant:
   Value : 1.61E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000110-86-1 Name: PYRIDINE

```
*******************************************************************************
MELT    PYRIDINE                                                CAS#   110-86-1
  Melting Point  :  -41.55      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      PYRIDINE                                                CAS#   110-86-1
  Vapor Pressure :  20.76       MM HG       MEAS
  Temperature (C):  25
  Abbrev. Ref.   :  CHAO,J ET AL. (1983)
*******************************************************************************

VP      PYRIDINE                                                CAS#   110-86-1
  Vapor Pressure :  20.8        MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

CHAO,J ET AL. (1983)
CHAO,J.; LIN,C.T.; CHUNG,T.H.; VAPOR PRESSURE OF COAL CHEMICALS.; J. PHYS. CHEM. REF. DATA.; 12:1033-63.; 1983

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000111-15-9 Name: ETHYLENE GLYCOL MONOETHYL ETHER ACETATE

```
*******************************************************************************
VP      ETHYLENE GLYCOL MONOETHYL ETHER ACETATE           CAS#   111-15-9
  Vapor Pressure :  2.340E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000111-15-9
Chem Name  : ETHOXYETHYLACETATE
Mol Formula: C6H12O3
Mol Weight : 132.16
Melting Pt : -61.7 deg C
Boiling Pt : 156.4 deg C
Water Solubility:
   Value : 2.47E+005 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.59
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 2.34 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.2E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : JOHANSON,G & DYNESIUS,B (1988)
Atmospheric OH Rate Constant:
   Value : 1.3E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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CHEMFATE Search Results

Return to EFDB page

CAS #: 000111-44-4 Name: BIS(2-CHLOROETHYL) ETHER

```
*****************************************************************************
MELT     BIS(2-CHLOROETHYL) ETHER                          CAS#   111-44-4
  Melting Point  :  -46.8        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************

VP       BIS(2-CHLOROETHYL) ETHER                          CAS#   111-44-4
  Vapor Pressure :  1.55         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*****************************************************************************
```

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

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Return to EFDB page

CAS #: 000111-44-4 Name: BIS(2-CHLOROETHYL) ETHER

```
*******************************************************************************
MELT    BIS(2-CHLOROETHYL) ETHER                              CAS#   111-44-4
  Melting Point  :  -46.8       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      BIS(2-CHLOROETHYL) ETHER                              CAS#   111-44-4
  Vapor Pressure :  1.55        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************
```

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI
AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY
WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000111-76-2 Name: 2-BUTOXYETHANOL

```
*******************************************************************************
MELT    2-BUTOXYETHANOL                                        CAS#   111-76-2
  Melting Point  :  -75          DEG C
  Remarks        :  MELTING POINT GIVEN IS REFERENCED AS FREEZING POINT, SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      2-BUTOXYETHANOL                                        CAS#   111-76-2
  Vapor Pressure :  .88E 00      TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  DORIGAN,J ET AL. (1976B)
*******************************************************************************

VP      2-BUTOXYETHANOL                                        CAS#   111-76-2
  Vapor Pressure :  0.88         MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  DOW CHEMICAL COMPANY (1981)
*******************************************************************************

VP      2-BUTOXYETHANOL                                        CAS#   111-76-2
  Vapor Pressure :  0.867        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

DORIGAN,J ET AL. (1976B)
DORIGAN,J.; FULLER,B.; DUFFY,R.; PRELIMINARY SCORING OF SELECTED ORGANIC AI POLLUTANTS. APPENDIX I - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS A THROUGH C.; EPA-450/3-77-008B. RESEARCH TRIANGLE PARK,NC: U.S. EPA PP.331. 1976B

DOW CHEMICAL COMPANY (1981)
DOW CHEMICAL COMPANY.; THE GLYCOL ETHERS HANDBOOK.; MIDLAND, MI: DOW CHEMICAL CO.; 1981

RIDDICK,JA ET AL. (1986)

RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000111-91-1 Name: BIS(2-CHLOROETHOXY)METHANE

```
*****************************************************************************
MELT     BIS(2-CHLOROETHOXY)METHANE                          CAS#   111-91-1
  Melting Point  :  -32          DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SAX,NI & LEWIS,RJSR (1987)
*****************************************************************************

VP       BIS(2-CHLOROETHOXY)METHANE                          CAS#   111-91-1
  Vapor Pressure :  1.4E-4       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE, EXTRAPOLATED FROM DATA IN THE RANGE
                    58-215 DEG C
  Abbrev. Ref.   :  PERRY,RH ET AL. (1984)
*****************************************************************************
```

PERRY,RH ET AL. (1984)
PERRY,R.H.; GREEN,D.W.; MALONEY,J.O.; PERRY'S CHEMICAL ENGINEERS' HANDBOOK; MCGRAW HILL; CRAWFORD & ECKES EDS.; 1984

SAX,NI & LEWIS,RJSR (1987)
SAX,N.I.; LEWIS,R.J.S.R.; HAWLEY'S CONDENSED CHEMICAL DICTIONARY 11TH ED; VANNOSTRAND REINHOLD CO.; N.Y.,N.Y.:P496; 1987

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 001120-71-4 Name: 2,2-DIOXIDE-1,2-OXATHIOLANE

```
*******************************************************************************
MELT    2,2-DIOXIDE-1,2-OXATHIOLANE                          CAS#  1120-71-4
  Melting Point  :  95.68       DEGC
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      2,2-DIOXIDE-1,2-OXATHIOLANE                          CAS#  1120-71-4
  Vapor Pressure :  17          MM HG       CALC
  Temperature (C):  25
  Remarks        :  CALC USING ESTIMATED HENRY'S LAW CONSTANT X WSOL, SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (NA--)
*******************************************************************************


   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

   SRC (NA--)
   SRC; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES.;   NA--

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000121-69-7 Name: N,N-DIMETHYLANILINE

```
*******************************************************************************
MELT    N,N-DIMETHYLANILINE                                   CAS#   121-69-7
  Melting Point  :  2.45        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      N,N-DIMETHYLANILINE                                   CAS#   121-69-7
  Vapor Pressure :  0.518       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CHAO,J ET AL. (1983)
*******************************************************************************

VP      N,N-DIMETHYLANILINE                                   CAS#   121-69-7
  Vapor Pressure :  7.000E-01   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

CHAO,J ET AL. (1983)
CHAO,J.; LIN,C.T.; CHUNG,T.H.; VAPOR PRESSURE OF COAL CHEMICALS.; J. PHYS. CHEM. REF. DATA.; 12:1033-63.; 1983

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

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CAS #: 000122-39-4 Name: DIPHENYLAMINE

```
*******************************************************************************
MELT    DIPHENYLAMINE                                          CAS#   122-39-4
  Melting Point  :  53-54       DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DEAN,JA (1985)
*******************************************************************************

VP      DIPHENYLAMINE                                          CAS#   122-39-4
  Vapor Pressure :  8.06E-4     MM HG       CALC
  Temperature (C):  20
  Remarks        :  EXTRAPOLATED FROM THE EXPERIMENTAL TEMPERATURE RANGE OF
                    62-397 DEG C
  Abbrev. Ref.   :  CHAO,J ET AL. (1983)
*******************************************************************************

VP      DIPHENYLAMINE                                          CAS#   122-39-4
  Vapor Pressure :  6.68E-4     MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  JONES,AH (1960)
*******************************************************************************
```

CHAO,J ET AL. (1983)
CHAO,J.; LIN,C.T.; CHUNG,T.H.; VAPOR PRESSURE OF COAL CHEMICALS.; J. PHYS. CHEM. REF. DATA.; 12:1033-63.; 1983

DEAN,JA (1985)
DEAN,J.A.; LANGE'S HANDBOOK OF CHEMISTRY 13TH ED.; NY, NY: MCGRAW-HILL BOO CO.; 1985

JONES,AH (1960)
JONES,A.H.; SUBLIMATION-PRESSURE DATA FOR ORGANIC COMPOUNDS.; J. CHEM. ENG. DATA.; 5:196-200.; 1960

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Diphenylhydrazine, 1,2-
CAS Number: 000122-66-7

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:		mg/kg/day	
Oral Slope:	8.0E-1	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:	8.0E-1	(mg/kg/day)^-1	HEAST
Inhal Wt-of-Evid:	B2		
Oral ED10:	2.3E-1	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B1		
Inhal ED10:	2.3E-1	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B1		
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.3E+2	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.4E+2	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	2.3E+1	days	THOMAS
Photolysis:		days	
Biodeg:	1.8E+2	days	FATERATE
Radio:		days	
Log Kow:	2.9E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.8E+2	
Density:	1.2E+0	g/mL @ 16.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	4.3E-4	Torr	CHEMFATE
Henry's Law:	1.5E-6	atm-m3/mol	CHEMFATE
Water Solub:	6.8E+1	mg/L	CHEMFATE
Distrib Coef:	1.2E+2	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	2.9E+0		CHEMFATE
Water Solub:	6.8E+1		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	1.3E+2	C
Boiling Point:		C
Formula:	C12 H12 N2	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000122-66-7 Name: 1,2-DIPHENYLHYDRAZINE

```
*****************************************************************************
MELT    1,2-DIPHENYLHYDRAZINE                                CAS#   122-66-7
  Melting Point  :  123-126     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*****************************************************************************

VP      1,2-DIPHENYLHYDRAZINE                                CAS#   122-66-7
  Vapor Pressure :  3.63E-5     MM HG       CALC
  Temperature (C):  25
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************

VP      1,2-DIPHENYLHYDRAZINE                                CAS#   122-66-7
  Vapor Pressure :  4.31E-4     MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*****************************************************************************
```

ALDRICH (1988)
ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI: ALDRICH CHEM CO.; 1988

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000123-33-1 Name: MALEIC HYDRAZIDE

```
*****************************************************************************
MELT    MALEIC HYDRAZIDE                                    CAS#   123-33-1
  Melting Point  :  306-308     DEG C
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ALDRICH (1988)
*****************************************************************************
```

ALDRICH (1988)
ALDRICH.; CATALOG HANDBOOK OF FINE CHEMICALS 1988-1989; MILWAUKEE, WI:
ALDRICH CHEM CO.; 1988

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000123-33-1
Chem Name  : MALEIC HYDRAZIDE
Mol Formula: C4H4N2O2
Mol Weight : 112.09
Melting Pt : 306 deg C
Boiling Pt :
Water Solubility:
   Value : 4510 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : TOMLIN,C (1994)
Log P (octanol-water):
   Value : -0.84
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 2.77E-006 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value : 5.67
   Temp  : 25 deg C
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 2.65E-011 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.33E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000144-62-7
Chem Name  : OXALIC ACID
Mol Formula: C2H2O4
Mol Weight : 90.04
Melting Pt : 189.5 dec deg C
Boiling Pt :
Water Solubility:
   Value : 2.2E+005 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : -2.22
   Type  : EST
   Ref   : JABER,HM ET AL. (1984)
Vapor Pressure:
   Value : 0.000234 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BARNALES,CA ET AL. (1981)
pKa Dissociation Constant:
   Value : 1.25
   Temp  :
   Type  :
   Ref   : BUXTON,GV ET AL. (1988)
Henry's Law Constant:
   Value : 1.43E-010 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : GAFFNEY,JS ET AL. (1987)
Atmospheric OH Rate Constant:
   Value : 7.2E-014 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : ATKINSON,R ET AL. (1988)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 025013-15-4
Chem Name  : VINYLTOLUENE
Mol Formula: C27H30
Mol Weight : 354.54
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 89 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LEWIS,PJ ET AL. (1978)
Log P (octanol-water):
   Value : 3.44
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 1.5 mm Hg
   Temp  : 20 deg C
   Type  : EXP
   Ref   : WEBER,RC ET AL. (1981)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.00262 atm-m3/mole
   Temp  : 20 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 5.34E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 041851-50-7
Chem Name  : 5-CHLORO-1,3-CYCLOPENTADIENE
Mol Formula: C5H5Cl
Mol Weight : 100.55
Melting Pt :
Boiling Pt :
Water Solubility:
   Value : 970 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 2.43
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 20.4 mm Hg
   Temp  : 25 deg C
   Type  : EST
   Ref   : NEELY,WB & BLAU,GE (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0224 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.42E-010 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

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CAS #: 000051-79-6 Name: ETHYL CARBAMATE

```
*******************************************************************************
MELT    ETHYL CARBAMATE                                          CAS#    51-79-6
  Melting Point  :  48-50        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      ETHYL CARBAMATE                                          CAS#    51-79-6
  Vapor Pressure :  0.76         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE, ESTIMATED USING PCCHEM BASED ON A
                    MP=49 DEG C & BP=183 DEG C
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000532-27-4 Name: 2-CHLORO-1-PHENYLETHANONE

```
*****************************************************************************
MELT     2-CHLORO-1-PHENYLETHANONE                          CAS#   532-27-4
  Melting Point  :  58-59        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP       2-CHLORO-1-PHENYLETHANONE                          CAS#   532-27-4
  Vapor Pressure :  5.4E-3       MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

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CAS #: 000540-73-8 Name: 1,2-DIMETHYLHYDRAZINE

```
*******************************************************************************
MELT    1,2-DIMETHYLHYDRAZINE                                   CAS#   540-73-8
  Melting Point  :  -85          DEG C
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      1,2-DIMETHYLHYDRAZINE                                   CAS#   540-73-8
  Vapor Pressure :  69.9         MM HG       MEAS
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  ASTON,JG ET AL. (1951)
*******************************************************************************
```

ASTON,JG ET AL. (1951)
ASTON,J.G.; JANZ,G.J.; RUSSELL,K.E.; THE HEAT CAPACITY, HEATS OF FUSION AND VAPORIZATION, VAPOR PRESSURES, AND ENTROPY OF SYMMETRICAL DIMETHYLHYDRAZINE J. AM. CHEM. SOC.; 73:1943-5; 1951

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

CHEMFATE Search Results

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CAS #: 000542-88-1 Name: BIS(CHLOROMETHYL) ETHER

```
*******************************************************************************
MELT     BIS(CHLOROMETHYL) ETHER                                CAS#   542-88-1
  Melting Point  :  -41.5        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HAWLEY,GG (1981)
*******************************************************************************

VP       BIS(CHLOROMETHYL) ETHER                                CAS#   542-88-1
  Vapor Pressure :  30           MM HG
  Temperature (C):  22
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************
```

CALLAHAN,MA ET AL. (1979A)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS-VOLUME II.; EPA-440/4-79-029 WASHINGTON,DC: U.S. EPA.; 1979A

HAWLEY,GG (1981)
HAWLEY,G.G.; THE CONDENSED CHEMICAL DISTIONARY. 10TH ED.; NEW YORK,NY: VAN NOSTRAND REINHOLD CO. PP.1135.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000057-14-7 Name: 1,1-DIMETHYLHYDRAZINE

```
*****************************************************************************
MELT    1,1-DIMETHYLHYDRAZINE                                CAS#    57-14-7
  Melting Point  :  -57.2       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SCHIESSL,HW (1980)
*****************************************************************************

VP      1,1-DIMETHYLHYDRAZINE                                CAS#    57-14-7
  Vapor Pressure :  157         MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SCHIESSL,HW (1980)
*****************************************************************************
```

SCHIESSL,HW (1980)
SCHIESSL,H.W.; HYDRAZINE AND ITS DERIVATIVES.; KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. NY,NY: WILEY-INTERSCIENCE. 12:734-71; 1980

End of Search

CHEMFATE Search Results

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CAS #: 000584-84-9 Name: 2,4-TOLUENE DIISOCYANATE

```
*****************************************************************************
MELT     2,4-TOLUENE DIISOCYANATE                          CAS#    584-84-9
  Melting Point  :  19.5-21.5   DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP       2,4-TOLUENE DIISOCYANATE                          CAS#    584-84-9
  Vapor Pressure :  0.008       MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*****************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

End of Search

CHEMFATE Search Results

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CAS #: 000059-89-2 Name: N-NITROSOMORPHOLINE

```
*****************************************************************************
MELT    N-NITROSOMORPHOLINE                                  CAS#    59-89-2
  Melting Point  :  29          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  IARC (1978)
*****************************************************************************

VP      N-NITROSOMORPHOLINE                                  CAS#    59-89-2
  Vapor Pressure :  3.6E-2      MM HG
  Temperature (C):  20
  Remarks        :  EXTRAPOLATED FROM 96 DEG C AT 6 MM HG, SRC RECOMMENDED VAL
  Abbrev. Ref.   :  KLEIN,RG (1982)
*****************************************************************************
```

IARC (1978)
IARC; MONOGRAPHS ON THE EVALUATION OF THE CARCINOGENIC RISK TO HUMANS. VOL.17. SOME N-NITROSO COMPOUNDS.; LYON,FRANCE: INTERNATIONAL AGENCY FOR RESEARCH ON CANCER.; 1978

KLEIN,RG (1982)
KLEIN,R.G.; CALCULATIONS AND MEASUREMENTS ON THE VOLATILITY OF N-NITROSAMIN AND THEIR AQUEOUS SOLUTIONS.; TOXICOLOGY; 23:135-47; 1982

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000060-34-4 Name: METHYLHYDRAZINE

```
*******************************************************************************
MELT    METHYLHYDRAZINE                                          CAS#    60-34-4
  Melting Point  :  -52.4       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      METHYLHYDRAZINE                                          CAS#    60-34-4
  Vapor Pressure :  .4906E 02   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  STONE,DA (1979)
*******************************************************************************

VP      METHYLHYDRAZINE                                          CAS#    60-34-4
  Vapor Pressure :  .496E 02    TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  SCHIESSL,HW (1980)
*******************************************************************************

VP      METHYLHYDRAZINE                                          CAS#    60-34-4
  Vapor Pressure :  50          MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BOUBLIK,T ET AL. (1984)
*******************************************************************************
```

BOUBLIK,T ET AL. (1984)
BOUBLIK,T.; FRIED,V.; HALA,E.; THE VAPOR PRESSURES OF PURE SUBSTANCES: SELECTED VALUES OF THE TEMPERATURE DEPENDENCE OF THE VAPOUR PRESSURES OF SO PURE SUBSTANCES IN THE NORMAL AND LOW PRESSURE REGION. VOL. 17.; AMSTERDAM NETHERLANDS: ELSEVIER SCI. PUBL.; 1984

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

SCHIESSL,HW (1980)
SCHIESSL,H.W.; HYDRAZINE AND ITS DERIVATIVES.; KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. NY,NY: WILEY-INTERSCIENCE. 12:734-71; 1980

STONE,DA (1979)
STONE,D.A.; THE AUTOOXIDATION OF MONOMETHYLHYDRAZINE VAPOR.; AFESC/ESL-TR-79-10. (NTIS AD-A069 173). TYNDALL AFB,FL: AIR FORCE ENG.

SERVICES CTR. PP.50.; 1979

End of Search

CHEMFATE Search Results

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CAS #: 000621-64-7 Name: N-NITROSO-DI-N-PROPYLAMINE

```
*****************************************************************************
MELT    N-NITROSO-DI-N-PROPYLAMINE                          CAS#   621-64-7
  Melting Point  :  7          DEGC
  Remarks        :  ESTIMATED BY EQUATION 20 IN NEELY,WB & BLAU,GE (1985), SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************

VP      N-NITROSO-DI-N-PROPYLAMINE                          CAS#   621-64-7
  Vapor Pressure :  0.13       MM HG
  Temperature (C):  25
  Remarks        :  ESTIMATED VALUE BASED ON A MEASURED VP OF 5 MM HG AT 81 DE
                    C, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KLEIN,RG (1982)
*****************************************************************************


   KLEIN,RG (1982)
   KLEIN,R.G.; CALCULATIONS AND MEASUREMENTS ON THE VOLATILITY OF N-NITROSAMIN
   AND THEIR AQUEOUS SOLUTIONS.; TOXICOLOGY; 23:135-47; 1982

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

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CAS #: 000062-50-0 Name: ETHYL METHANESULFONATE

```
*******************************************************************************
MELT     ETHYL METHANESULFONATE                                  CAS#     62-50-0
  Melting Point  :  -0.41        DEGC
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP       ETHYL METHANESULFONATE                                  CAS#     62-50-0
  Vapor Pressure :  0.206        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  JABER,HM ET AL. (1984B)
*******************************************************************************
```

JABER,HM ET AL. (1984B)
JABER,H.M.; MABEY,W.R.; LIU,A.T.; CHOU,T.W.; JOHNSON,H.L.; DATA AQUISITION FOR ENVIRONMENTAL TRANSPORT AND FATE SCREENING FOR COMPOUNDS OF INTEREST TO THE OFFICE OF EMERGENCY AND REMEDIAL RESPONCE.; EPA-600/6-84-011. (NTIS PB84-245281). MENLO PARK,CA: SRI INTERNATIONAL. PP.156.; 1984B

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000627-13-4
Chem Name  : 1-PROPYLNITRATE
Mol Formula: C3H7NO3
Mol Weight : 105.09
Melting Pt : -100 deg C
Boiling Pt : 110 deg C
Water Solubility:
   Value : 3290 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HAUFF,K ET AL. (1998)
Log P (octanol-water):
   Value : 1.74
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 23.5 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BOUBLIK,T ET AL. (1984)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.00127 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : HAUFF,K ET AL. (1998)
Atmospheric OH Rate Constant:
   Value : 7.3E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : KWOK,ESC & ATKINSON,R (1994)
```

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CHEMFATE Search Results

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CAS #: 000062-75-9 Name: DIMETHYLNITROSAMINE

```
*****************************************************************************
MELT    DIMETHYLNITROSAMINE                                  CAS#    62-75-9
  Melting Point  :  -50         DEGC
  Remarks        :  SRC RECOMMENDED VALUE, ESTIMATED BY PCCHEM-PCGEMS
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************

VP      DIMETHYLNITROSAMINE                                  CAS#    62-75-9
  Vapor Pressure :  2.7         MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KLEIN,RG (1982)
*****************************************************************************
```

KLEIN,RG (1982)
KLEIN,R.G.; CALCULATIONS AND MEASUREMENTS ON THE VOLATILITY OF N-NITROSAMIN AND THEIR AQUEOUS SOLUTIONS.; TOXICOLOGY; 23:135-47; 1982

SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000065-85-0
Chem Name  : BENZOIC ACID
Mol Formula: C7H6O2
Mol Weight : 122.12
Melting Pt : 122.4 deg C
Boiling Pt : 249.2 deg C
Water Solubility:
   Value : 3400 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.87
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.0007 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : MCEACHERN,DM & SANDOVAL,O (1973)
pKa Dissociation Constant:
   Value : 4.19
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LIDE,DR (1996)
Henry's Law Constant:
   Value : 3.81E-008 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.24E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CAS #: 000077-78-1 Name: DIMETHYL SULFATE

```
*******************************************************************************
MELT    DIMETHYL SULFATE                                        CAS#    77-78-1
  Melting Point  :  -27          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      DIMETHYL SULFATE                                        CAS#    77-78-1
  Vapor Pressure :  0.68         MM HG
  Temperature (C):  20
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  WEBER,RC ET AL. (1981)
*******************************************************************************
```

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

WEBER,RC ET AL. (1981)
WEBER,R.C.; PARKER,P.A.; BOWSER,M.; VAPOR PRESSURE DISTRIBUTION OF SELECTED ORGANIC CHEMICALS.; EPA-600/2-81-021. CINCINNATI,OH: U.S.EPA. PP.39.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000079-10-7 Name: ACRYLIC ACID

```
*******************************************************************************
MELT    ACRYLIC ACID                                          CAS#    79-10-7
  Melting Point  :  13.5        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      ACRYLIC ACID                                          CAS#    79-10-7
  Vapor Pressure :  4.00        MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

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CAS #: 000085-44-9 Name: PHTHALIC ANHYDRIDE

```
*****************************************************************************
VP      PHTHALIC ANHYDRIDE                                  CAS#    85-44-9
  Vapor Pressure :  5.17E-4     MM HG
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM 30 DEG C, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  JONES,AH (1960)
*****************************************************************************
```

JONES,AH (1960)
JONES,A.H.; SUBLIMATION-PRESSURE DATA FOR ORGANIC COMPOUNDS.; J. CHEM. ENG. DATA.; 5:196-200.; 1960

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here.
References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000085-44-9
Chem Name  : PHTHALIC ANHYDRIDE
Mol Formula: C8H4O3
Mol Weight : 148.12
Melting Pt : 130.8 deg C
Boiling Pt : 295 deg C
Water Solubility:
   Value : 6200 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : TOWLE,PH ET AL. (1968)
Log P (octanol-water):
   Value : 1.60
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.000517 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : JONES,AH (1960)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 1.63E-008 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 7.49E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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CHEMFATE Search Results

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CAS #: 000090-04-0 Name: O-METHOXYANILINE

```
*****************************************************************************
MELT    O-METHOXYANILINE                                        CAS#    90-04-0
  Melting Point  :  5           DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*****************************************************************************

VP      O-METHOXYANILINE                                        CAS#    90-04-0
  Vapor Pressure :  0.08        MM HG
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM PERRY, GREEN 1984 - 61 TO 132 DEG C, SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************

VP      O-METHOXYANILINE                                        CAS#    90-04-0
  Vapor Pressure :  8.000E-02   MM HG       EXTRAPOLATED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  PERRY,RH & GREEN,D (1984)
*****************************************************************************


   MERCK INDEX (1983)
   MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH
   ED.;  WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

   PERRY,RH & GREEN,D (1984)
   PERRY,R.H.; GREEN,D.; PERRY'S CHEMICAL HANDBOOK. PHYSICAL AND CHEMICAL DATA
    NEW YORK,NY: MCGRAW HILL. 6TH ED.; 1984

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

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7 CAS #: 000091-22-5 Name: QUINOLINE

```
*******************************************************************************
MELT    QUINOLINE                                          CAS#    91-22-5
  Melting Point  :  -14.85      DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      QUINOLINE                                          CAS#    91-22-5
  Vapor Pressure :  0.096       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  CHAO,J ET AL. (1983)
*******************************************************************************

VP      QUINOLINE                                          CAS#    91-22-5
  Vapor Pressure :  6.000E-02   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

CHAO,J ET AL. (1983)
CHAO,J.; LIN,C.T.; CHUNG,T.H.; VAPOR PRESSURE OF COAL CHEMICALS.; J. PHYS. CHEM. REF. DATA.; 12:1033-63.; 1983

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

CHEMFATE Search Results

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CAS #: 000924-16-3 Name: DI(N-BUTYL)NITROSAMINE

```
*****************************************************************************
MELT    DI(N-BUTYL)NITROSAMINE                                CAS#   924-16-3
  Melting Point  :  2.13        DEGC
  Remarks        :  ESTIMATED BY PCCHEM-PCGEMS, SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SRC (1988)
*****************************************************************************

VP      DI(N-BUTYL)NITROSAMINE                                CAS#   924-16-3
  Vapor Pressure :  3.0E-2      MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  KLEIN,RG (1982)
*****************************************************************************


   KLEIN,RG (1982)
   KLEIN,R.G.; CALCULATIONS AND MEASUREMENTS ON THE VOLATILITY OF N-NITROSAMIN
   AND THEIR AQUEOUS SOLUTIONS.; TOXICOLOGY; 23:135-47; 1982

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000092-52-4 Name: BIPHENYL

```
*******************************************************************************
MELT    BIPHENYL                                                CAS#    92-52-4
  Melting Point  :  69-71       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      BIPHENYL                                                CAS#    92-52-4
  Vapor Pressure :  .975E-1     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  UNITS CONVERTED
  Abbrev. Ref.   :  WEAVER,WC ET AL. (1979)
*******************************************************************************

VP      BIPHENYL                                                CAS#    92-52-4
  Vapor Pressure :  .58E-01     TORR        MEASURED
  Temperature (C):  25.
  Remarks        :  FROM MACKAY,D. & WOLKOFF,A.W. (1973)
  Abbrev. Ref.   :  KILZER,L ET AL. (1979)
*******************************************************************************

VP      BIPHENYL                                                CAS#    92-52-4
  Vapor Pressure :  8.93E-3     MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  BURKHARD,LP ET AL. (1984)
*******************************************************************************

VP      BIPHENYL                                                CAS#    92-52-4
  Vapor Pressure :  9.64E-03    MM HG
  Temperature (C):  25
  Remarks        :  VALUE EXTRAPOLATED FROM DATA FOR THE SOLID MATERIAL OVER
                    10-60 DEG C. SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  SASSE,K ET AL. (1989)
*******************************************************************************
```

BURKHARD,LP ET AL. (1984)
BURKHARD,L.P.; ARMSTRONG,D.E.; ANDREN,A.W.; VAPOR PRESSURES FOR BIPHENYL, 4-CHLOROBIPHENYL, 2,2',3,3',5,5',6,6'-OCTACHLOROBIPHENYL, AND DECACHLOROBIPHENYL.; J. CHEM. ENG. DATA.; 29:248-50.; 1984

KILZER,L ET AL. (1979)
KILZER,L.; SCHEUNERT,I.; GEYER,H.; KLEIN,W.; KORTE,F.; LABORATORY SCREENING OF THE VOLATILIZATION RATES OF ORGANIC CHEMICALS FROM WATER AND SOIL.; CHEMOSPHERE.; 8:751-61.; 1979

MERCK INDEX (1983)
MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH ED.; WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

SASSE,K ET AL. (1989)
SASSE,K.; N'GUIMBI,J.; JOSE,J.; MERLIN,J.C.; VAPOR PRESSURE OF POLYAROMATIC HYDROCARBONS IN THE 10 -3 TO 10 TORR RANGE.; THERMOCHIM. ACTA.; 146:53-61; 1989

WEAVER,WC ET AL. (1979)
WEAVER,W.C.; SIMMONS,P.B.; THOMPSON,Q.E.; DIPHENYL AND TERPHENYLS.; IN: KIRK-OTHMER ENCYL. CHEM. TOXICOL. 3RD ED. 7:782-93.; 1979

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000094-59-7 Name: SAFROLE

```
*******************************************************************************
MELT    SAFROLE                                                CAS#    94-59-7
  Melting Point  :  11.2        DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DEAN,JA (1985)
*******************************************************************************

VP      SAFROLE                                                CAS#    94-59-7
  Vapor Pressure :  1.09E-1     MM HG       CALC
  Temperature (C):  25
  Remarks        :  ESTIMATED BY PCCHEM
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      SAFROLE                                                CAS#    94-59-7
  Vapor Pressure :  7.06E-2     MM HG       CALC
  Temperature (C):  25
  Remarks        :  EXTRAPOLATED FROM DATA OBTAINED IN THE RANGE 63.8-233 DEG
                    DATA TAKEN FROM PERRY & GREEN (1984). SRC RECOMMENDED VALU
  Abbrev. Ref.   :  OHE,S (1976)
*******************************************************************************


   DEAN,JA (1985)
   DEAN,J.A.; LANGE'S HANDBOOK OF CHEMISTRY 13TH ED.;  NY, NY: MCGRAW-HILL BOO
   CO.; 1985

   OHE,S (1976)
   OHE,S.; COMPUTER AIDED DATA BOOK OF VAPOR PRESSURE.;  DATA BOOK PUBL. CO.,
   TOKYO, JAPAN.; 1976

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000096-45-7 Name: ETHYLENETHIOUREA

```
*******************************************************************************
MELT    ETHYLENETHIOUREA                                        CAS#    96-45-7
  Melting Point  :  203-204     DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  MERCK INDEX (1983)
*******************************************************************************

VP      ETHYLENETHIOUREA                                        CAS#    96-45-7
  Vapor Pressure :  5.85E-7     MM HG       CALC
  Temperature (C):  25
  Remarks        :  ACCURACY UNCERTAIN, ESTIMATED PCCHEM
  Abbrev. Ref.   :  SRC (1988)
*******************************************************************************

VP      ETHYLENETHIOUREA                                        CAS#    96-45-7
  Vapor Pressure :  1.4E-04     MM HG       CALC
  Temperature (C):  25
  Remarks        :  CALC FROM ESTIMATED HENRY'S LAW CONSTANT AND ESTIMATED WSO
                    SRC RECOMMENDED VALUE.
  Abbrev. Ref.   :  SRC (NA--)
*******************************************************************************


   MERCK INDEX (1983)
   MERCK INDEX.; THE MERCK INDEX. AN ENCYCLOPEDIA OF CHEMICALS AND DRUGS 10TH
   ED.;  WINDHOLZ,M ED. RAHWAY, N.J.: MERCK AND CO., INC.; 1983

   SRC (1988)
   SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES;   1988

   SRC (NA--)
   SRC; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES.;   NA--

End of Search
```

CHEMFATE Search Results

Return to EFDB page

CAS #: 000098-01-1 Name: FURFURAL

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*******************************************************************************
VP      FURFURAL                                                CAS#    98-01-1
  Vapor Pressure :  2.210E+00   MM HG       MEASURED
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

End of Search

Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value.
References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000098-01-1
Chem Name  : FUFURAL
Mol Formula: C5H4O2
Mol Weight : 96.09
Melting Pt : -36.5 deg C
Boiling Pt : 161.7 deg C
Water Solubility:
   Value : 7.7E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 0.41
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 2.21 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 3.37E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 3.51E-011 cm3/molecule-sec
   Temp  : 27 deg C
   Type  : EXP
   Ref   : BIERBACH,A ET AL. (1995)
```

Back To PhysProp Demo Page

CHEMFATE Search Results

Return to EFDB page

CAS #: 000098-86-2 Name: ACETOPHENONE

```
*******************************************************************************
MELT    ACETOPHENONE                                          CAS#    98-86-2
  Melting Point  :  19.62       DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP      ACETOPHENONE                                          CAS#    98-86-2
  Vapor Pressure :  .3715E 00   TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  DREISBACH,RR (1955)
*******************************************************************************

VP      ACETOPHENONE                                          CAS#    98-86-2
  Vapor Pressure :  0.397       MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1985)
*******************************************************************************
```

DAUBERT,TE & DANNER,RP (1985)
DAUBERT,T.E.; DANNER,R.P.; DATA COMPILATION TABLES OF PROPERTIES OF PURE COMPOUNDS.; AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. PP.450; 1985

DREISBACH,RR (1955)
DREISBACH,R.R.; PHYSICAL PROPERTIES OF CHEMICAL COMPOUNDS. I.; ADVANCES IN CHEMISTRY SERIES NO. 15.; WASHINGTON, DC: AMERICAN CHEMICAL SOCIETY.; 1955

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

WTP RISK ASSESSMENT WORK PLAN IDENTIFIED CONSTITUENTS OF POTENTIAL CONCERN (COPC) SUPPORT DATA

Phthalates (PHT)

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Bis (2-ethylhexyl) phthalate
CAS Number: 000117-81-7

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	2.0E-2	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:	1.4E-2	(mg/kg/day)^-1	IRIS
Oral Wt-of-Evid:	B2		
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:	5.2E+0	mg/kg/day	EPA_ED10
Oral ED10 Wgt:	B2		
Inhal ED10:	5.2E+0	mg/kg/day	EPA_ED10
Inhal ED10 Wgt:	B2		
Oral LD50:	2.6E+4	mg/kg	ACGIH
Dermal LD50:	2.5E+4	mg/kg	ACGIH
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.6E+2	µg/L	ECOTOX
Salt Ecol LC50:	1.0E+3	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	7.3E+5	days	CHEMFATE
Volatility:	6.9E+2	days	THOMAS
Photolysis:	2.0E+2	days	FATERATE
Biodeg:	8.0E-1	days	CHEMFATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	7.3E+5	days	CHEMFATE
Volatility:	4.8E+2	days	THOMAS
Photolysis:	2.0E+2	days	FATERATE
Biodeg:	8.0E-1	days	CHEMFATE
Radio:		days	
Log Kow:	5.1E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	3.9E+2	
Density:	9.8E-1	g/mL @ 25.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	6.8E-8	Torr	CHEMFATE
Henry's Law:	1.0E-7	atm-m3/mol	CHEMFATE
Water Solub:	3.4E-1	mg/L	CHEMFATE
Distrib Coef:	2.3E+6	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	2.1E+4		ECOTOX
Salt BCF:	2.7E+2		ECOTOX
ENVIRONMENTAL			
Fresh BCF:	1.1E+5		ECOTOX
Salt BCF:	6.5E+3		ECOTOX
Log Kow:	5.1E+0		CHEMFATE
Water Solub:	3.4E-1		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-5.5E+1	C
Boiling Point:	3.8E+2	C
Formula:	C24 H38 O4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000117-81-7 Name: DI(2-ETHYLHEXYL)PHTHALATE

```
*******************************************************************************
MELT     DI(2-ETHYLHEXYL)PHTHALATE                                CAS#   117-81-7
  Melting Point  :  -50          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  RIDDICK,JA ET AL. (1986)
*******************************************************************************

VP       DI(2-ETHYLHEXYL)PHTHALATE                                CAS#   117-81-7
  Vapor Pressure :  .62E-07      TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  GIAM,CS ET AL. (1980)
*******************************************************************************

VP       DI(2-ETHYLHEXYL)PHTHALATE                                CAS#   117-81-7
  Vapor Pressure :  .2E-06       TORR        MEASURED
  Temperature (C):  20.
  Abbrev. Ref.   :  CALLAHAN,MA ET AL. (1979A)
*******************************************************************************

VP       DI(2-ETHYLHEXYL)PHTHALATE                                CAS#   117-81-7
  Vapor Pressure :  6.45E-6      MM HG
  Temperature (C):  25
  Abbrev. Ref.   :  HOWARD,PH ET AL. (1985)
*******************************************************************************

VP       DI(2-ETHYLHEXYL)PHTHALATE                                CAS#   117-81-7
  Vapor Pressure :  6.78E-08     MM HG
  Temperature (C):  25
  Remarks        :  VALUE EXTRAPOLATED FROM DATA FROM 25-88 DEG C. SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  DAUBERT,TE & DANNER,RP (1989)
*******************************************************************************
```

CALLAHAN,MA ET AL. (1979A)
CALLAHAN,M.A.; SLIMAK,M.W.; GABEL,N.W.; MAY,I.P.; FOWLER,C.F.; FREED,J.R.; JENNINGS,P.; DURFEE,R.L.; WHITMORE,F.C.; MAESTRI,B. ET AL.; WATER-RELATED ENVIRONMENTAL FATE OF 129 PRIORITY POLLUTANTS-VOLUME II.; EPA-440/4-79-029 WASHINGTON,DC: U.S. EPA.; 1979A

DAUBERT,TE & DANNER,RP (1989)
DAUBERT,T.E.; DANNER, R.P.; PHYSICAL AND THERMODYNAMIC PROPERTIES OF PURE CHEMICALS: DATA COMPILATION.; DESIGN INSTITUTE FOR PHYSICAL PROPERTY DATA, AMERICAN INSTITUTE OF CHEMICAL ENGINEERS. HEMISPHERE PUB. CORP., NEW YORK, NY., 4 VOL.; 1989

GIAM,CS ET AL. (1980)
GIAM,C.S.; ATLAS,E.; CHAN,H.S.; NEFF,G.S.; PHTHALATE ESTERS, PCB, AND DDT RESIDUES IN THE GULF OF MEXICO ATMOSPHERE.; ATMOS. ENVIRON.; 14:65-9.; 1980

HOWARD,PH ET AL. (1985)
HOWARD,P.H.; BANERJEE,S.; ROBRILLARD,K.H.; MEASUREMENT OF WATER SOLUBILITIE OCTANOL-WATER PARTITION COEFFICIENTS AND VAPOR PRESSURES OF COMMERCIAL PHTHALATE ESTERS.; ENVIRON. TOX. CHEM.; 4:653-61.; 1985

RIDDICK,JA ET AL. (1986)
RIDDICK,J.A.; BUNGER,W.B.; SAKANO,T.K.; ORGANIC SOLVENTS: PHYSICAL PROPERTI AND METHODS OF PURIFICATION.; TECHNIQUES OF CHEMISTRY. 4TH ED. NEW YORK,NY WILEY-INTERSCIENCE. 2:PP.1325; 1986

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Di-n-octyl phthalate
CAS Number: 000117-84-0

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	2.0E-2	mg/kg/day	HEAST
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:	5.0E+3	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:		µg/L	
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.9E+2	days	CHEMFATE
Volatility:	1.7E+2	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.9E+2	days	CHEMFATE
Volatility:	2.6E+0	days	THOMAS
Photolysis:		days	
Biodeg:	2.8E+1	days	FATERATE
Radio:		days	
Log Kow:	8.1E+0		PHYSPROP

PHYSICAL CHARACTERISTICS

Parameter	Value		
Metal Contain:	No		
Organic:	Yes		
Gas:	Yes		
Particulate:	Yes		
Radionuclide:	No		
Rad. Element:	No		
Molecular Weight:	3.9E+2		
Density:		g/mL @	C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	2.6E-6	Torr	CHEMFATE
Henry's Law:	6.7E-5	atm-m3/mol	CHEMFATE
Water Solub:	2.0E-2	mg/L	CHEMFATE
Distrib Coef:	1.3E+7	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	1.1E+2		VER_BCF
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	2.9E+4		ECOTOX
Salt BCF:			
Log Kow:	8.1E+0		PHYSPROP
Water Solub:	2.0E-2		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	2.5E+1	C
Boiling Point:		C
Formula:	C24 H38 O4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000117-84-0 Name: DI-N-OCTYL PHTHALATE

```
*****************************************************************************
MELT    DI-N-OCTYL PHTHALATE                                CAS#   117-84-0
  Melting Point  :  -25         DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BEMIS,AG ET AL. (1982)
*****************************************************************************

VP      DI-N-OCTYL PHTHALATE                                CAS#   117-84-0
  Vapor Pressure :  2.6E-6      MM HG
  Temperature (C):  25
  Remarks        :  NOT CLEAR IF VALUE IS EXPERIMENTAL OR EXTRAPOLATED, SRC
                    RECOMMENDED VALUE
  Abbrev. Ref.   :  PERWAK,J ET AL. (1981)
*****************************************************************************
```

BEMIS,AG ET AL. (1982)
BEMIS,A.G.; DINDORF,J.A.; HORWOOD,B.; SAMANS,C.; PHTHALIC ACIDS, AND OTHER BENZENEPOLYCARBOXYLIC ACIDS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 17:732-77.; 1982

PERWAK,J ET AL. (1981)
PERWAK,J.; GOYER,M.; SCHIMKE,G.; ESCHENROEDER,A.; FIKSEL,J.; EXPOSURE AND RISK ASSESSMENT FOR PHTHALATE ESTERS (DI(2-ETHYLHEXYL)PHTHALATE, DI-N-BUTYL PHTHALATE, DIMETHYL PHTHALATE, DIETHYL PHTHALATE, DI-N-OCTYL PHTHALATE, BUT BENZYL PHTHALATE) (REVISED).; EPA-440/4-81-020. (NTIS PB85-211936). CAMBRIDGE,MA: ARTHUR D. LITTLE INC. PP.176.; 1981

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000131-11-3 Name: DIMETHYL PHTHALATE

```
*******************************************************************************
MELT    DIMETHYL PHTHALATE                                    CAS#   131-11-3
  Melting Point  :  0-2          DEGC
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  BEMIS,AG ET AL. (1982)
*******************************************************************************

VP      DIMETHYL PHTHALATE                                    CAS#   131-11-3
  Vapor Pressure :  0.00165      MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HOWARD,PH ET AL. (1985)
*******************************************************************************
```

BEMIS,AG ET AL. (1982)
BEMIS,A.G.; DINDORF,J.A.; HORWOOD,B.; SAMANS,C.; PHTHALIC ACIDS, AND OTHER BENZENEPOLYCARBOXYLIC ACIDS.; IN: KIRK-OTHMER ENCYCL. CHEM. TECH. 3RD ED. 17:732-77.; 1982

HOWARD,PH ET AL. (1985)
HOWARD,P.H.; BANERJEE,S.; ROBRILLARD,K.H.; MEASUREMENT OF WATER SOLUBILITIE OCTANOL-WATER PARTITION COEFFICIENTS AND VAPOR PRESSURES OF COMMERCIAL PHTHALATE ESTERS.; ENVIRON. TOX. CHEM.; 4:653-61.; 1985

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Diethyl phthalate
CAS Number: 000084-66-2

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	8.0E-1	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	9.5E+3	mg/kg	ACGIH
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.2E+4	µg/L	ECOTOX
Salt Ecol LC50:	4.9E+3	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.2E+3	days	FATERATE
Volatility:	2.2E+2	days	THOMAS
Photolysis:		days	
Biodeg:	5.6E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.2E+3	days	FATERATE
Volatility:	8.3E+1	days	THOMAS
Photolysis:		days	
Biodeg:	5.6E+1	days	FATERATE
Radio:		days	
Log Kow:	2.5E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.2E+2	
Density:	1.2E+0	g/mL @ 14.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	1.6E-3	Torr	CHEMFATE
Henry's Law:	4.5E-7	atm-m3/mol	CHEMFATE
Water Solub:	1.1E+3	mg/L	CHEMFATE
Distrib Coef:	4.4E+1	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	1.2E+2		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	2.1E+2		ECOTOX
Salt BCF:			
Log Kow:	2.5E+0		CHEMFATE
Water Solub:	1.1E+3		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-4.1E+1	C
Boiling Point:	3.0E+2	C
Formula:	C12 H14 O4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000084-66-2 Name: DIETHYL PHTHALATE

```
*******************************************************************************
VP      DIETHYL PHTHALATE                                    CAS#    84-66-2
  Vapor Pressure :  .35E-03     TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  EXTRAP, UNITS CONVERTED, RANGE OF MEASUREMENTS 34-61 DEGC
  Abbrev. Ref.   :  GRAYSON,BT & FOSBRAEY,LA (1982)
*******************************************************************************

VP      DIETHYL PHTHALATE                                    CAS#    84-66-2
  Vapor Pressure :  1.65E-3     MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HOWARD,PH ET AL. (1985)
*******************************************************************************
```

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End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Di-n-butyl phthalate
CAS Number: 000084-74-2

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	1.0E-1	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	8.0E+0	mg/kg	RTECS
Dermal LD50:	2.1E+4	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	2.8E+2	µg/L	ECOTOX
Salt Ecol LC50:	2.0E+1	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:	3.7E+3	days	CHEMFATE
Volatility:	1.7E+2	days	THOMAS
Photolysis:	1.4E+2	days	FATERATE
Biodeg:	2.3E+1	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:	3.7E+3	days	CHEMFATE
Volatility:	2.4E+1	days	THOMAS
Photolysis:	1.4E+2	days	FATERATE
Biodeg:	2.3E+1	days	FATERATE
Radio:		days	
Log Kow:	4.7E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	2.8E+2	
Density:	1.0E+0	g/mL @ 20.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	7.3E-5	Torr	CHEMFATE
Henry's Law:	1.8E-6	atm-m3/mol	CHEMFATE
Water Solub:	1.1E+1	mg/L	CHEMFATE
Distrib Coef:	5.2E+3	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	6.7E+3		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	8.8E+3		ECOTOX
Salt BCF:	2.3E+3		ECOTOX
Log Kow:	4.7E+0		CHEMFATE
Water Solub:	1.1E+1		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	-3.5E+1	C
Boiling Point:	3.4E+2	C
Formula:	C16 H22 O4	

CLASS INFORMATION

Class	Parent Substance

CHEMFATE Search Results

Return to EFDB page

CAS #: 000084-74-2 Name: DIBUTYL PHTHALATE

```
*****************************************************************************
VP      DIBUTYL PHTHALATE                                   CAS#    84-74-2
  Vapor Pressure :  .14E-04     TORR        MEASURED
  Temperature (C):  25.
  Abbrev. Ref.   :  GIAM,CS ET AL. (1980)
*****************************************************************************

VP      DIBUTYL PHTHALATE                                   CAS#    84-74-2
  Vapor Pressure :  .1E-01      TORR        MEASURED
  Temperature (C):  20.
  Remarks        :  UPPER LIM
  Abbrev. Ref.   :  MARTIN,H & WORTHING,CR (1977)
*****************************************************************************

VP      DIBUTYL PHTHALATE                                   CAS#    84-74-2
  Vapor Pressure :  7.3E-5      MM HG
  Temperature (C):  25
  Remarks        :  SRC RECOMMENDED VALUE
  Abbrev. Ref.   :  HOWARD,PH ET AL. (1985)
*****************************************************************************
```

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MARTIN,H.; WORTHING,C.R.; PESTICIDE MANUAL. FIFTH EDITION, BRITISH CROP PROTECTION COUNCIL. 563 PP.; 1977

End of Search

CHEMFATE Search Results

Return to EFDB page

CAS #: 000085-68-7 Name: BUTYL BENZYL PHTHALATE

```
*******************************************************************************
MELT    BUTYL BENZYL PHTHALATE                                  CAS#    85-68-7
  Remarks          :  NO APPROPRIATE ESTIMATION METHOD
  Abbrev. Ref.     :  SRC (1988)
*******************************************************************************

MELT    BUTYL BENZYL PHTHALATE                                  CAS#    85-68-7
  Melting Point    :  -35          DEG C
  Remarks          :
              1    :  CRYSTALLIZING POINT, GIVEN AS < VALUE
              2    :   BAYER AG INTERNAL DATA
              3    :   HPV: PHTHALATE ESTERS
  Abbrev. Ref.     :  US EPA (2004)
*******************************************************************************

VP      BUTYL BENZYL PHTHALATE                                  CAS#    85-68-7
  Vapor Pressure :  0.19E+01     TORR         MEASURED
  Temperature (C):  200.
  Abbrev. Ref.     :  GLEDHILL,WE ET AL. (1980)
*******************************************************************************

VP      BUTYL BENZYL PHTHALATE                                  CAS#    85-68-7
  Vapor Pressure :  8.25E-6      MM HG
  Temperature (C):  25
  Remarks          :  SRC RECOMMENDED VALUE
  Abbrev. Ref.     :  HOWARD,PH ET AL. (1985)
*******************************************************************************
```

GLEDHILL,WE ET AL. (1980)
GLEDHILL,W.E.; KALEY,R.G.; ADAMS,W.J.; HICKS,O.; MICHAEL,P.R.; SAEGER,V.W.; LEBLANC,G.A.; AN ENVIRONMENTAL SAFETY ASSESSMENT OF BUTYL BENZYL PHTHALATE. ENVIRON. SCI. TECH.; 14:301-5.; 1980

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SRC (1988)
SRC.; SYRACUSE RESEARCH CORPORATION CALCULATED VALUES; 1988

US EPA (2004)
U.S. EPA; HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM. THE HPV VOLUNTARY CHALLENGE CHEMICAL LIST. ROBUST SUMMARIES AND TEST PLANS.; WASHINGTON, DC:

USEPA, OFF. PREVENT. PEST. TOX. SUBST., POLLUT. PREVENT. TOXICS. AVAILABLE HTTP://WWW.EPA.GOV/OPPTINTR/CHEMRTK/HPVCHMLT.HTM AS OF MARCH, 2004.; 2004

End of Search

SUPERFUND CHEMICAL DATA MATRIX

Date: 1/28/2004
Chemical: Butylbenzyl phthalate
CAS Number: 000085-68-7

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:	2.0E-1	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	2.3E+3	mg/kg	RTECS
Dermal LD50:	1.0E+4	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	6.8E+2	µg/L	ECOTOX
Salt Ecol LC50:	4.6E+2	µg/L	ECOTOX

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.9E+2	days	THOMAS
Photolysis:	1.0E+2	days	CHEMFATE
Biodeg:	4.0E+0	days	CHEMFATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	3.6E+1	days	THOMAS
Photolysis:	1.0E+2	days	CHEMFATE
Biodeg:	4.0E+0	days	CHEMFATE
Radio:		days	
Log Kow:	4.9E+0		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value		
Metal Contain:	No		
Organic:	Yes		
Gas:	Yes		
Particulate:	Yes		
Radionuclide:	No		
Rad. Element:	No		
Molecular Weight:	3.1E+2		
Density:		g/mL @	C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	8.3E-6	Torr	CHEMFATE
Henry's Law:	1.3E-6	atm-m3/mol	CHEMFATE
Water Solub:	2.7E+0	mg/L	CHEMFATE
Distrib Coef:	8.7E+3	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:	7.7E+2		ECOTOX
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	7.7E+2		ECOTOX
Salt BCF:			
Log Kow:	4.9E+0		CHEMFATE
Water Solub:	2.7E+0		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:		C
Boiling Point:		C
Formula:	C19 H20 O4	

CLASS INFORMATION

Class	Parent Substance

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Appendix H

Organic Abatement DFs in Pretreatment PVP System

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Appendix H
Organic Abatement DFs in Pretreatment PVP System

Appendix H provides the methodology used to determine the organic constituents decontamination factors through the pretreatment vessel vent system thermal oxidizer and carbon beds. The numbers provided are conservative and provide bounding conditions for the emissions profile analysis.

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Appendix H

Pretreatment Vessel Vent Organic Constituents Decontamination Factor Analysis

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List of Acronyms

Acronym	Description
AIT	auto ignition temperature
CAS #	Chemical Abstract Service registry number
COPC	constituent of potential concern
DE	destruction efficiency
DF	decontamination factor
EPA	US Environmental Protection Agency
LFL	lower flammability limit
MSDS	material safety data sheet
MW	molecular weight
PCBs	poly-chlorinated biphenyls
ppmv	part per million by volume
PT	pretreatment
PVP	pretreatment vessel vent process system
RTO	regenerative thermal oxidizer
RE	removal efficiency
VLE	vapor-liquid equilibrium
VOC	volatile organic compound
WTP	Hanford Tank Waste Treatment and Immobilization Plant

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1 Objective

The objective of this analysis is to determine the decontamination factors (DFs) for abatement of potential organic constituents in the pretreatment (PT) vessel vent process (PVP) system.

2 Existing Design Inputs

2.1 RTO Design Criteria

Conditions of combustion within the regenerative thermal oxidizer (RTO) unit are 1.0 second residence time at 1600 °F according to the *System Description for Pretreatment Vessel Vent Process System, PVP* (24590-PTF-3YD-PVP-00001).

2.2 Carbon Adsorber Design Criteria

Carbon adsorbers are designed to contain the largest volume of carbon media possible within the limits of pressure drop and facility size limitations for exchanging spent adsorbers with freshly charged adsorbers (24590-PTF-M0C-PVP-00003).

3 Background

3.1 Origins of Organic Compounds in the PVP System

Historical characterization of Hanford tank waste shows various organic compounds in the solids, liquids, and headspace vapors of numerous double- and single-shelled tanks. Organic solvents and complexants were used in nuclear fuel processing and account for the bulk of the original organic material sent to the waste tanks. Since then, complex reactions have taken place where the original organic waste compounds have undergone radiolytic decomposition to form other compounds. The decomposition products can continuously change in composition since many of them are reactive with other organic decomposition products or may undergo further radiolytic decay. The sustained radioactive exposure to original organic waste material accounts for potentially thousands of different organic compounds present in the waste at trace quantities.

Waste batches will be sent from Hanford tank farms to the Hanford Tank Waste Treatment and Immobilization Plant (WTP) PT facility for processing prior to vitrification. While in PT, process vessels are swept with forced and passive air purges to ensure that radiolytically generated hydrogen does not concentrate in vessel headspaces to a flammable level. The sweeping of process vessel headspaces allows for the removal of organic compounds as governed by the vapor-liquid equilibrium (VLE) of each compound at the system conditions.

3.2 Organic Abatement in the PVP System

Air purges from PT process vessels are removed and treated through the PVP system prior to discharge to the environment. To ensure that the concentration of volatile organic compounds (VOCs) in the PT offgas is reduced before release to the environment, the stream is processed through an RTO and a carbon adsorber. In the RTO, organic compounds are destroyed via combustion. The combustion reaction is induced by the application of high temperature and the availability of excess oxygen. Destruction of

contaminants is followed by a polishing step in the adsorber where some removal of remaining organic compounds takes place. In the adsorber, organic contaminants are removed from the vent gas by capture on the surface of the activated carbon media.

3.3 Organic Characterization of Hanford Tank Wastes

Due to the difficulties associated with sample handling and analysis of radioactive tank waste, the organic characterization of waste liquid and solids remains largely incomplete with respect to the species and concentration of each organic compound. The most abundant organic characterization data comes from tank headspace analyses. A wide range of target organic compounds have been detected in various tank headspace samples on behalf of the relative ease of vapor phase sample handling during analysis. Over 1200 different organic compounds have been detected through historical sampling and analyses of Hanford tank wastes (Wiemers 1998 p 4.13). Nearly all 1200 of these compounds have been detected in the headspace samples of single-shell tanks (Stock 2000, p 2).

In spite of the organic analysis data available to date, there is still significant uncertainty in determining the potential concentrations of the individual and collective organic compounds within the PVP system vent stream. Arguably, organic concentrations will be appreciably lower in the PVP system vent gas than detected concentrations from historical headspace analysis. Most of the data was collected several years ago and since then the organic compounds have continued to be depleted by ventilation of the waste tanks. However, those compounds which have been detected at higher concentrations are generally the most credible in terms of their presence in multiple tanks. As such, the organic compounds most likely to be detectable in the PVP system vent gas are those which have been detected in some abundance in several different waste tanks.

3.4 Constituents of Potential Concern

In this integrated emissions baseline report, 219 organic constituents of potential concern (COPCs) were identified as being relevant to emissions estimates for permitting. These 219 COPCs were identified during development of the *Environmental Risk Assessment Work Plan for the Hanford Tank Waste Treatment and Immobilization Plant* (24590-WTP-RPT-ENS-03-006). These constituents have been included in emissions estimates used for permitting the WTP. As such, they are also considered in this analysis to establish conservative DFs to be included when determining future emissions estimates used in permitting activities.

Of the 219 COPCs, 14 are coplanar poly-chlorinated biphenyls (PCBs). These 14 PCBs are included individually in the list on due to the tendency for the coplanar molecules to exhibit dioxin-like properties. The specific PCBs are shown in addition to the generally identified compound, PCB (Chemical Abstract Service [CAS] # 1336-36-3), which is inclusive of the entire family of individual PCBs.

3.5 Organic Destruction via Combustion –Theory

Thermal oxidation of organic material is a combustion process. Combustion is defined as the burning of gases, liquids, or solids, in which the substance is oxidized, evolving heat and often light (Lewandowski 2000, p 1). For combustion to occur, three elements of the reaction need to be in place. These are fuel (the organic contaminant in this case), oxygen (present in the vent gas, which is mostly air), and an ignition source. The ignition source can be thought of as the source of activation energy to initiate the chemical (combustion) reaction. In general, combustion reactions are exothermic and under the correct conditions of oxygen and fuel, initiated combustion can release enough heat to sustain a continuous ignition source (the burning process or a "fire"). The following chemical equation shows the products of combustion for a typical hydrocarbon.

Equation H-1

$$C_xH_{2y} + \left(X + \frac{Y}{2}\right)O_2 + Q_{activation} \rightarrow XCO_2 + YH_2O + Q_{combustion}$$

where:

X and Y	= stoichiometric coefficients
C	= carbon
H	= hydrogen
CO_2	= carbon dioxide combustion product
H_2O	= water vapor combustion product
$Q_{activation}$	= activation energy to initiate the reaction
$Q_{combustion}$	= combustion energy released by forming the combustion products

Within a thermal oxidation system, the primary performance requirement is the extent of destruction or destruction efficiency (DE) of the organic contaminants. Important parameters which affect the DE of organics by thermal oxidation are sometimes called the "three T's" of combustion. The "T's" are time, temperature, and turbulence. The other most important parameter is availability of oxygen. The extent of oxygen present in a combustion system essentially determines the importance of time and turbulence. As the availability of oxygen increases, the need for time and turbulence (mixing) will decrease for the same DE since there is more likelihood for the same number of contaminants to contact and react with an oxygen molecule. Typically, thermal oxidizers use a fuel supply and burner system to maintain the system operating temperature. In such cases, the excess oxygen is usually managed to levels which are only slightly higher than the stoichiometric requirement. The reason for limiting the excess oxygen is a cost consideration which limits the fuel required to maintain the system temperature (fuel efficiency). In systems where oxygen is rigorously controlled, time and turbulence become a vital design consideration to ensure equivalent DE.

The PVP system will use an RTO which will maintain operating temperature by heat input from an electric element as opposed to a burner system. In this service, the extent of excess oxygen is very near 20.9 % (the oxygen concentration in ambient air) since the organic contaminants in the PVP system stream are expected to be extremely dilute. The RTO will recover energy from the high temperature exhaust by exchanging heat with (preheating) the feed gas via ceramic heat transfer beds. Oxidizers which use ceramic heat transfer beds in alternating flow cycles are known as *regenerative*. This manner of heat recovery will maximize the energy efficiency of the oxidizer and provide some additional residence time at temperatures very near the operating temperature.

The design parameters required for the PVP system oxidizer are 1.0 second residence time at 1600 °F. This is consistent with US Environmental Protection Agency (EPA) reported results of commercial incinerators (fuel-fired) where 0.75 seconds and 1600 °F have been shown to ensure DEs remain above 98 % for non-halogenated VOCs (EPA 1999, p 1). Additionally, electric heating elements used in existing RTOs have demonstrated proven reliability when operating at 1500 °F and the capability of operating as high as 1800 °F. It should be noted that the EPA reference which states destruction performance for this operating temperature has derived the information from historical performance of fired oxidizers (as opposed to electric). The reference states the importance of mixing and residence time in this type of system since the availability of oxygen is limited by the system's operationally practical fuel efficiency.

3.6 Organic Removal via Adsorption – Theory

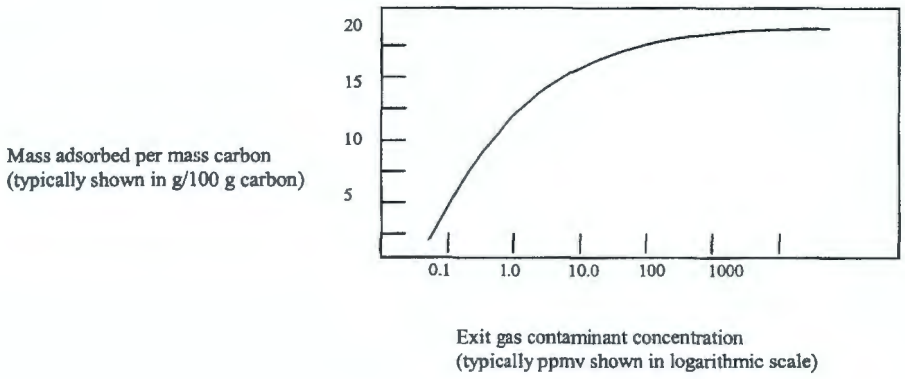
The adsorption of VOCs on activated carbon media occurs by a physical adsorption mechanism in which weak attractive forces, resulting from Van der Waals forces between the contaminant and the carbon adsorbent (also known as Hydrogen bonding forces or London dispersion forces) adhere the contaminant to the surface of the carbon. The process is exothermic and usually evolves slightly more energy than the heat of vaporization of the adsorbed compound (Cooper 1994, p 381). The contaminant essentially moves out of the vapor phase to behave like a liquid or solid phase trapped on the solid surface of the adsorbent media. Adsorption is usually reversible. Under appropriate sustained conditions of temperature, pressure, and concentration, most adsorbed compounds can re-enter the vapor phase as governed by thermodynamic equilibrium.

In general, the potential for activated carbon to adsorb a particular contaminant depends primarily on the boiling point and molecular weight (MW) of that compound. The reason is that some molecules tend to have more potential for intermolecular attraction via London dispersion forces. A generally predictive measure of intermolecular forces is normal boiling point since the change of phase requires enough energy to break the intermolecular forces which hold the compound together in its liquid phase. A higher boiling point corresponds with a higher intermolecular attraction (Brown 1994, p 374) and hence more potential for strong adsorption. Consequently, boiling point is the strongest indicator for the "adsorbability" of a particular VOC. Boiling point is followed closely by MW as an indicator of adsorption potential. Large molecules with large MWs tend to have more atoms and therefore more potential to be polarized. The polar characteristic of a molecule adds to the attractive forces due to the pull between dissimilar charges. The more "polarizable" a molecule is, the more intermolecular force it exhibits and hence the more adsorbable it may be.

3.6.1 Adsorption Isotherms

Adsorption is governed by thermodynamics of chemical equilibrium; therefore, contaminant concentration in the treated gas is an important factor in determining the capacity of the carbon to collect or load a particular constituent. Temperature and pressure conditions also affect the extent of adsorption so that higher pressure and lower temperature favor a higher adsorption capacity. This is consistent with the observation that gas phase adsorption is exothermic at essentially the latent heat of vaporization. The adsorption behaves like a phase change; both high pressure and low temperature favor this transition. At constant pressure and temperature, the relationship between contaminant concentration in the exit gas and the equilibrium capacity of the adsorbent is known as an adsorption isotherm.
, below, depicts a generalized relationship between carbon loading capacity and equilibrium exit gas concentration.

Figure H-1



Isotherms are empirically created from experimental or industrial data and are commonly available for numerous VOCs on adsorbents developed for several types of gas cleaning services. However, at extremely dilute concentrations, the predictive capability of empirically developed isotherms becomes unreliable. The reason is that adsorption data is not widely available at extremely low concentrations since there is not normally a regulatory driver to apply adsorption technology to significantly dilute streams. Industrial experience suggests that adsorption capacities for dilute contaminant concentrations should be determined through pilot testing of each adsorbent media considered for the service. The performance or removal efficiency (RE) of activated carbon will vary depending on media particle size, type of activation processing (internal pore size, pore distribution, or void fraction), and carbon source material.

3.6.2 Multi-Component Adsorption

In multi-component adsorption, the adsorption capacity of any particular compound may no longer follow its particular single compound isotherm. Complex and unpredictable component-to-component interactions may take place. This can change the thermodynamic equilibrium of the collective adsorption system. It is known, however, that in systems where a weakly attracted compound has been adsorbed, it can later be displaced by a more strongly adsorbed compound if the relative concentrations favor the exchange. This "selective" behavior greatly adds to the complexity and unpredictability of multi-component adsorption.

Processing of each batch of Hanford tank waste is likely to evolve multiple species of VOCs at dilute concentrations, each with its own unique organic signature. In the case where potentially hundreds of different organic compounds may be present at different concentrations, the contaminants will be competing for the same adsorption sites. The prediction of equilibrium for any given compound becomes virtually impossible. Given the unpredictable mix of compounds and concentrations in the PVP system vent gas, those compounds which are only slightly adsorbable are not likely to exhibit any appreciable removal from the stream.

3.7 Compound Physical Property Sources

The list of contaminants considered by this analysis includes compounds detected through various historical analyses of Hanford tank wastes and those considered due to regulatory concern. These compounds exhibit a wide range of physical properties. Not all of the relevant physical property values were found to be readily available. For the most part, chemistry and engineering handbooks and texts have been referenced to supply the important physical properties used in this analysis. In addition, several Internet databases containing information on chemical compounds, chemistry, and chemical safety were used to further complete the collection of physical properties. In some cases, manufacturer's material safety data sheets (MSDS) were used to provide the auto-ignition temperatures (AITs), solubilities, and/or boiling points of certain compounds.

This group of sources, however, did not provide all of the required information for every compound. To fill the remaining gaps, comparisons were made to similar compounds for which data was found. The missing physical property information was then conservatively estimated. Primarily, chemical structure was used to assign AITs and normal boiling points. To a lesser extent, molecular weight, solubility, and National Fire Prevention Association hazard rankings were taken into consideration. General chemical trends were accounted for when assessing the conservatism of each estimated value. Examples of trends include: 1) the polarity of a compound with respect to estimated boiling point and 2) the number of halogen substitutions, chemical resonance, or length of alkane chain with respect to estimated AIT.

3.8 Representative Organic Compounds

Given the total number of historically detected organic compounds which could be considered for tracking through the PVP system, a criteria was needed to select a smaller and more manageable number of representative compounds. The "representative" compounds will include organic COPCs identified by the *Environmental Risk Assessment Work Plan for the Hanford Tank Waste Treatment and Immobilization Plant*. The organic COPCs contain numerous halogenated and aromatic compounds which appear at the extreme ends of the range of physical property values used to assign DFs. The representative compounds can then bound the behavior of those which may not be tracked in the PVP system. By including several compounds which are difficult to destroy or remove from the PVP system vent gas, future emissions estimates can establish bounding conservatism by assigning higher concentrations to these low abated compounds.

Since the compounds under consideration are those which may be present within the PVP system vent gas, the considerable data collected from headspace (vapor) samples of the single-shell tanks was considered to be the widest and most representative information. A single source document containing the maximum detected concentration of nearly 1200 compounds (Stock 2000) was used to set the selection criteria for some of the representative compounds. It is appropriate to include the organic COPCs in this analysis because of their inclusion in emissions estimates which affect WTP air permitting. The criteria for selecting the remaining compounds was decided to be a maximum detected concentration of 0.1 part per million by volume (ppmv) or higher.

Some of the compounds detected at 0.1 ppmv or higher are COPCs[1]. However, all tabular data presented in this analysis are shown as two lists: 1) the COPCs and 2) those detected over the concentration threshold. This is done to make it easier to locate particular compound information based on the different end uses expected from this analysis. The total number of individual compounds considered in this analysis is 405. Tables 1-1 and 1-2 of Attachment 1 show the COPCs and detected compounds in tank headspace, respectively.

All organic COPCs identified in the *Environmental Risk Assessment Work Plan for the Hanford Tank Waste Treatment and Immobilization Plant* will be included in this analysis with the exception of the individual coplanar PCBs. Due to the similarity of PCBs across all the various specific structures and physical properties, the 14 listed coplanar PCBs will not be treated individually in this analysis. Those compounds are assigned a single DF identified by the descriptive name (PCBs) and CAS # 1336-36-3.

3.9 Compound Physical Properties

Tables 1-1 and 1-2 show a CAS #, MW, chemical formula, boiling point, and AIT for each compound. A two-dimensional structure is also shown for each compound where the structure is not obvious by its compound name and/or where it is significant to the determination of any estimated physical property value. Values which could not be found in available references have been estimated as described in Section 3.7 of this analysis. Source information and notes concerning particular physical property values are included at the end of each table. As can be expected with such a large collection of data from several different sources, some values may be inconsistent with other sources. However, since conservatism has been exercised at each occurrence of estimation or enabling assumption, the individual and collective physical property inputs are considered to be bounding as supported by the best available information. As

[1] Not all of the COPCs have been detected in analysis of headspace samples of Hanford tank waste.

such, their effect on the analysis result with respect to the accuracy of assigned DFs is expected to be conservatively bounding.

3.10 Destruction Criteria

Section 2.1 gives the design conditions of residence time and operating temperature of the RTO. For a given constituent, the availability of oxygen and its AIT are the other important factors for determining DE in the RTO system.

3.10.1 Oxygen Concentration

Final vapor-liquid equilibrium (VLE) for organic compounds in the PVP system vent gas will take place in the caustic scrubber, which is controlled to near standard conditions. These conditions are essentially the same as waste tank storage conditions at the Hanford Site. Therefore, the expected concentration of organic compounds will be much less than 1 % since most volatile compounds have already been depleted from the waste. As such, the oxygen concentration of the vent gas is essentially that of saturated ambient air (>20 %) and is well in excess of typical combustion systems where excess oxygen is controlled for fuel efficiency.

3.10.2 Basis of Destruction

Given the design criteria of the RTO and the extent of available oxygen for combustion, the DF for destruction of each compound will be determined by its AIT. See Section 5.4 for a detailed explanation of AIT and the relationship of destruction efficiency in the RTO.

3.11 Removal Criteria

For assigning DFs across the carbon adsorber, normal boiling point, MW, and concentration are considered. It is understood that the concentration of any given constituent in the PVP system vent gas cannot be accurately predicted. However, some constituents are known to be extensively destroyed in the oxidizer, leaving a very small concentration in the feed gas to the downstream adsorber. This qualitative behavior is taken into consideration on those compounds which have high DFs across the RTO. For a detailed explanation of how boiling point, MW, and concentration are used to assign adsorber DFs, see Section 5.5.

4 Methodology

4.1 Definition of Decontamination Factor

The mathematical definition of decontamination factor (DF) is generally the ratio of mass flow in the feed to mass flow in the treated stream. DFs will be calculated by using the DE or RE in the following relationship.

Equation H-2

$$DF = \frac{1}{\left[1 - \frac{eff}{100}\right]}$$

where:

eff = the contaminant DE or RE in %

4.2 Destruction DF

Each compound's referenced or estimated AIT will be compared with the operating temperature of the RTO. The difference in these two temperatures will be used to assign a destruction DF based on the criteria from Table H-2.

4.3 Removal DF

Compound removal DFs across carbon adsorption will be assigned based on the estimated adsorption capacity of each compound. The estimated adsorption capacities are based on normal boiling point, molecular weight, and available calculated adsorption capacities (Yaws 1995) for certain compounds which are included in this analysis. Where the capacity estimation via molecular weight and normal boiling point differs from the calculated prediction for a specific compound, the lower value is used to ensure conservatism. For the 35 instances where the correlation gives the lower capacity estimate, the correlation value was rounded down to the nearest graduated capacity from Table H-3. The selected adsorption capacity is then used to assign the removal DFs according to Table H-4.

4.4 Combined DF

The carbon adsorption system normally treats gas that has been processed in the RTO. As such, the inlet concentration of certain constituents has the potential of being extremely low (<<0.1 ppmv for compounds which are readily combustible). The potential for extremely low contaminant concentrations will be accounted for by applying a reduction scalar on compounds which have a DF of 50 or higher across the RTO. For these compounds, the adsorption DF used to calculate the combined DF will be reduced by a factor of 10 (not to decrease below 1.0). The combined DF will then be determined by multiplication of the DFs for the RTO and carbon adsorber.

5 Assumptions

5.1 Physical Property Sources

Due to the number and species of the organic compounds considered by this analysis, not all physical property values were readily available. In addition, certain sources contradicted each other regarding AIT and normal boiling point. A good example of this is the chemical compound pyridine (CAS # 110-86-1). Physical property sources #1 and #6 from Table 1-2 show the normal boiling points to be 115.2 °C and 208 °C respectively. Another example is naphthalene (CAS # 91-20-3). Sources #1 and #23 from Table 1-2 show the AITs as 568 °C and 526 °C respectively. Likewise, numerous AIT temperatures were found by searching MSDS and chemical safety databases, and in some cases, two available sources showed different AITs. In all instances where differing values were found, the more conservative (high AIT and low boiling point) were used. However, due to the number of discrepancies found and the apparent potential for inaccuracy, the physical data has been treated with conservatism in determining the destruction and removal DFs. The physical property data as assembled in Tables 1-1 and 1-2 is assumed to be best available information and appropriate to determine combined DFs. This assumption (and any specific physical property value) is not unreasonable since the inaccuracy of the physical property data is not likely to significantly affect the combined DF of any compound. In addition, the DFs determined by this analysis are likely to be used with a very conservative estimation of unabated organic emissions due

to the uncertainty of organic content in the tank waste. In this manner, an estimation of abated organic emissions from the PT PVP system can be considered bounding.

5.2 Physical Property Values

Numerous uncommon organic species are contained within the collective compounds considered by this analysis. As not all physical properties were found for several of these compounds, the AIT and normal boiling point were estimated in some cases to enable the DFs to be assigned. As discussed in Section 3.7, the compound physical structures were used to estimate the AIT and/or boiling point by comparison to similar compounds for which the values were known. When estimating the AITs, certain trends related to elemental composition and chemical structure were recognized. In general, the following patterns are reflected in the reference AITs:

- Aromatics tend to have higher AITs due to resonance stability.
- Halogenated compounds have higher AITs.
- Higher carbon to halogen atomic ratios have lower AITs.
- Methyl or alkane substitutions of otherwise identical structures lowers the AIT.
- Compounds with longer alkane chains tend to have lower AITs.
- Carbon, nitrogen, or oxygen double bonds tend to raise AIT in most compounds.
- Higher hydrogen to carbon ratios tend to lower AIT temperature.

All of these trends were taken into consideration to ensure that the estimated AITs were bounded by conservatism. When estimating normal boiling point, more extreme conservatism was exercised to ensure that the lower boiling point compounds were reflected as lower than the actual value (resulting in conservative adsorption DF). At higher values of boiling point, the accuracy of the estimates becomes less important as the graduated categories for adsorption capacities are associated with wide ranges of boiling points. In many cases, the molecular weight of compounds with unknown boiling points were so high that the boiling points of similar structures were far in excess of the maximum criteria for assigning adsorption DF. On behalf of these measures of conservatism, the estimated physical properties which affect the destruction or removal are assumed to be bounding and their criteria will not contribute any non-conservative error to the assigned DFs.

5.3 Unidentified and Non-included Organic Compounds

It is assumed that previously unidentified or lesser detected compounds will behave similarly to the 400+ compounds considered by this analysis. The COPCs include an abundance of halogenated compounds which are most difficult to destroy in the thermal oxidizer. In addition, several of the halogenated compounds are methanes and ethanes (refrigerants) which have little or no adsorption potential. For this reason, the individual compounds considered by this analysis are assumed to conservatively represent the potential organic compounds which could be evolved from the waste. In order for an emissions estimate to establish a conservative bound for emissions, both the implementation of the DFs established by this analysis and a conservative estimate of organic compounds in the feed are required.

5.4 Destruction Efficiency

Time, turbulence, and temperature are commonly referred to as the most important factors on the extent of complete combustion in thermal oxidation or incineration abatement systems. The three "T's", however, do not specifically address the availability of oxygen (one of the components of the combustion

triangle). The reason is that most commonly the systems under consideration are fired with auxiliary fuel in some type of burner arrangement. In such cases, the oxygen content is usually regulated at a concentration slightly in excess of stoichiometric for the sake of fuel efficiency. Stoichiometric oxygen is typically limited at 3.0 volume percent in the exhaust gas of fired systems. Predictions of destruction efficiency in systems with limited oxygen are not based purely on temperature. The following sections discuss the basis for assigning combustion DFs in the PVP system.

5.4.1 Excess Oxygen

A general relationship between operating temperature, contaminant AIT, residence time, turbulence, percent excess oxygen in the exhaust gas, and DE has been developed and used in the design of incineration systems. Data showing the dependency of DE on temperature and residence time is shown in the table below (Lewandowski 2000 p 27).

Table H-1

Destruction Efficiency (%)	Degrees Above AIT (°F)	Residence Time (s)
95	300	0.5
98	400	0.5
99	475	0.75
99.9	550	1.0
99.99	650	2.0

The table shows DE as a function of the operating temperature in excess of contaminant AIT. This relationship assumes that a threshold turbulence (Reynolds number ≥10,000) and 3.0 % excess oxygen are achieved. The upper bound values given in the table suggest that not all of a contaminant is completely destroyed. Even at a temperature of 650 °F above the AIT of a contaminant, 0.01 % of the compound is shown to remain undestroyed in the stream.

Oxygen-starved pathways are presumed to be responsible for the un-combusted residual (Lewandowski 2000 p 26). A study of destruction mechanisms to help predict the DEs in oxygen-deficient systems was conducted by the EPA. The resulting EPA Incinerability Ranking was developed to provide relative destruction of compounds under oxygen-deficient conditions. The study and its results were published in an Environmental Science and Technology article entitled *Development of a Thermal Stability Based Ranking of Hazardous Organic Compound Incinerability* (Dellinger 1990). Various relationships were discussed in the article suggesting factors such as elemental composition of the contaminants and the potential for formation of reactive radicals are primary indicators of thermal stability (or instability). Figure 9 of the article shows a two-dimensional plot of temperature vs. the remaining fraction of contaminant (see Attachment 5) illustrating the effect of varying excess oxygen. Numerous data sets are plotted, each representing a different extent of excess oxygen (shown as oxygen equivalence ratio {stoichiometric oxygen/actual oxygen}). A dramatic separation occurs between the plots of oxygen equivalence ratios 1.0 and 1.001. With only the additional 1/1000 of stoichiometric oxygen provided when moving from the equivalence ratio of 1.001 to 1.0, equal destruction is achieved at a significantly lower temperature (more than 100 °C lower). In general, the plots all follow the trend of higher available oxygen equating to a lower temperature of equal destruction. However, the differences are subtle until the ratio drops below a value of 1.01. This established trend is a clear indication that oxygen content is the most significant variable to account for when determining destruction efficiency at temperatures above the AIT. As oxygen availability increases, the required temperature for equivalent destruction decreases toward the AIT.

5.4.2 Basis of Destruction

Based on the results shown in Figure 9 of Dellinger 1990, and the expected concentration of oxygen in the treated gas of the RTO, the contaminant AIT is assumed to be the single determining variable in assigning organic DFs. Considering the design residence time of 1.0 second under the conditions of excess oxygen in the PVP system vent gas (see Section 3.10.1), the DEs shown in Table H-1 are considered to be conservatively bounding and valid for assigning DFs in the PVP system RTO. In order to assign DFs at lower extents than what is shown in Table H-1, data points were extrapolated and fitted to a well-behaved plotted function (see trendline of Figure H-2 below). Table H-2 shows the data points for the DFs associated with each predicted destruction efficiency.

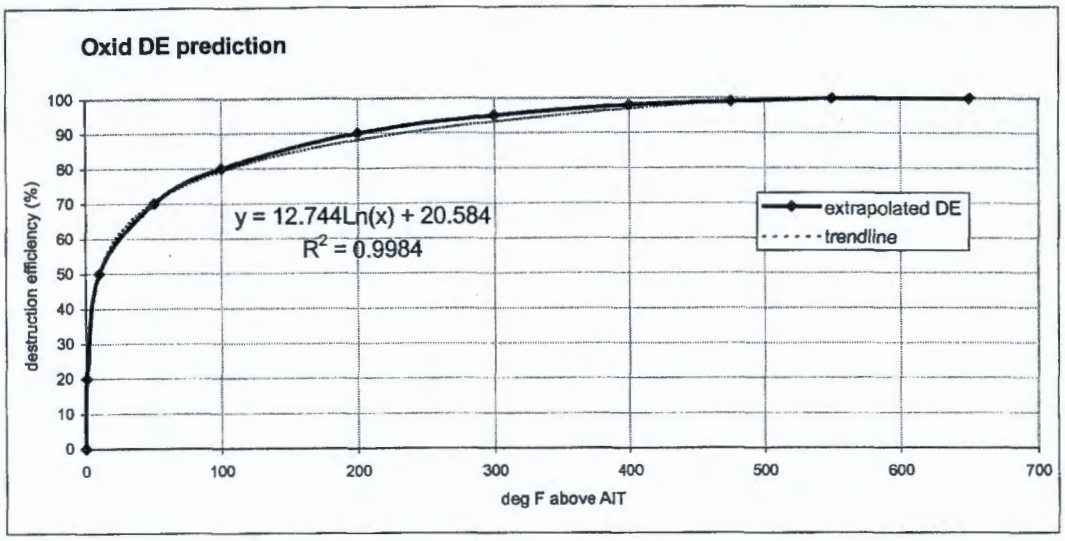
Table H-2

Degrees Above AIT (°F)	Destruction Efficiency (%)	DF (massflow in/massflow out)
<0.2	0	1
1	20	1.25
10	50	2
50	70	3.33
100	80	5
200	90	10
300	95	20
400	98	50
475	99	100
550	99.9	1000
≥650	99.99	10000

The data point for 0.2 °F at zero destruction efficiency is included for the sake of fitting the extrapolated data to the trend line on the plot and for establishing the lower boundary of DE at a conservative fixed point. Given the 1.0 second residence time at operating temperature, some destruction can be expected to take place at the AIT threshold. However, to remain conservative the DF assigned to compounds with AITs of higher than 1599 °F (operating temperature is 1600 °F) will be 1.0.

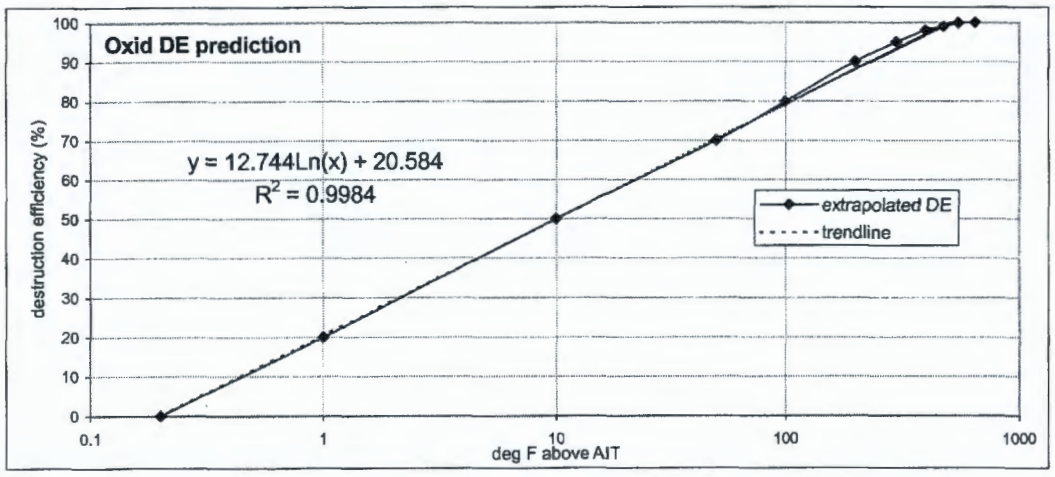
Figure H-2 shows the plotted data points on normal scale and Figure H-3 show the data on a logarithmic scale to better resolve the DE at temperatures just above the AIT.

Figure H-2



General behavior of the plot is reasonable for DE since one would expect the efficiency to be near zero at the initial occurrence of the AIT and then become appreciable rapidly as the temperature increases.

Figure H-3



The plot shown on logarithmic scale indicates that the prediction for destruction efficiency decreases to zero before the operating temperature decreases below the AIT.

While the extrapolation is not expected to be perfectly accurate for each compound, it does reflect reasonable behavior under the combustion conditions of the electric RTO. Given the conservatism applied in assigning AITs and the maximum extent of available oxygen in the treated stream, the DFs are assumed to be both appropriate and achievable.

5.4.3 Residence Time

The design residence time of 1.0 second is assumed to be adequate for all of the above AITs and associated DFs to be valid. This assumption is made while taking into consideration the data shown in

Table H-1. The DE of 99.99 % is shown for 650 °F above the AIT and a 2.0 second residence time. The extra second of residence time (2.0 seconds compared to 1.0 in this system) can be thought of as increasing the likelihood of small remaining amounts of contaminant finding available oxygen and reacting. Given that the data was derived from systems operating with 3.0 % excess oxygen, the increase to nearly 21 % oxygen (in this system) should more than compensate for the shortened residence time at equal predicted DE.

5.5 Removal Efficiency

The extent of removal for a contaminant depends on its adsorption potential and concentration. Adsorption potential can be estimated for individual compounds based on physical properties, provided the concentration of the contaminant is not dilute beyond the limits of isotherm data. Multi-component adsorption is much more difficult since contaminant interactions can be unpredictable. The organic signature of the PVP system vent gas will change throughout the operation of the WTP. As such, enabling assumptions are needed to assign individual adsorption potentials. Given that the adsorbers will be designed within the recommended gas loading rate of 10 to 100 ft/min (24590-PTF-M0C-PVP-00003), the following assumptions are conservatively bounding with respect to adsorption potential and removal DFs.

5.5.1 Equilibrium Gas Concentrations

No definitive information exists which can predict the concentration of an individual contaminant in the feed to the carbon adsorber. Arguably, the more volatile compounds may already be depleted from the waste due to the continuous removal by the ventilation systems of the waste tanks in the tank farm. Those which are not volatile enough to have already escaped from the tank waste are not likely to be volatile enough to be appreciably present in the PVP system due to the comparable conditions of temperature and pressure. Overall, the probability of any single constituent to exceed 0.1 ppmv in the adsorber feed is quite low. This presents difficulty when assigning adsorption capacity for any compound since adsorption technology is not traditionally applied to such dilute concentrations of contaminants. As such, little or no isotherm data are available for compounds at or below 0.1 ppmv.

To enable adsorption assignments, the exit gas concentration will be assumed to be 0.1 ppmv for each compound. This concentration is the lowest for which reference data can be reasonably extrapolated. Selecting this reference point will establish the best available comparison for use in assigning a conservative adsorption capacity for each contaminant from Tables 1-1 and 1-2.

5.5.2 Adsorption Capacity Estimate Methodology

As a starting point to consider the different adsorption potentials in this analysis, molecular weight and boiling point criteria from a technology paper on vapor phase carbon adsorption were used to set graduated thresholds of capacity. The paper, *Activated Carbon Adsorption for Treatment of VOC Emissions* (Shepherd 2001), provides relative adsorption capacities of several common organic compounds (see Attachment 6). The capacities exhibit the governing behavior of adsorption potential based primarily on boiling point and MW of each compound. From the relative capacities and trends shown by the compounds included in this source, the following table was developed to assign the graduated capacities for the same criteria of PVP system contaminants:

Table H-3

Contaminant Normal Boiling Point	Contaminant Molecular Weight	Estimated Adsorption Capacity
°C	g/mol	g adsorbed/100g carbon
<25	-	0
-	<50	0
25-50	<150	0.5
<50	-	1
50-100	<150	1
50-100	-	2
100-150	<150	2
100-150	-	5
>150	<150	10
150-200	-	20
>200	-	40

*Note: The dash (-) indicates all values are applicable, given that the compound is not classified by criteria from a previous row.

This graduated assignment of capacity may be too general with respect to compounds in a given classification of boiling point and MW since the property value ranges are large. Additionally, no reference is made to compound concentration within the relative capacities presented by the technology paper.

To qualify the values of Table H-3, the assigned capacities of several compounds were compared to the corresponding predicted results of a correlation equation. The equation was developed from available isotherm data of numerous organic compounds (Yaws 1995). The results for common organic compounds having four or fewer carbon atoms were obtained from a quadratic equation as a function each contaminant's assumed concentration and compound-specific quadratic coefficients (see Attachment 7). The logarithmic series expansion equation is shown below:

Equation H-3

$$\log_{10} Q = A + B \log_{10} y + C[\log_{10} y]^2$$

where:

Q = adsorption capacity at equilibrium (g/100 g carbon)
y = contaminant concentration in ppmv
A, B, and C = quadratic coefficients (contaminant specific)

Of the 405 compounds considered by this analysis, 95 were found to have coefficients for prediction of their adsorption capacity by this correlation. In general, the predicted results were in alignment with the estimated capacities assigned from Table H-3 criteria. However, the correlation capacity results were lower than the estimated capacities for 35 of the 95 compounds. The differences in predicted capacities (difference = correlation results – estimated capacity) ranged from –1.9 to 16 (g/100 g carbon). This

shows that the graduated capacities determined by the estimation method are generally conservative and in agreement with the correlation. For most compounds, the estimation method is well below the correlation result. It is assumed that the lower predicted capacity from either Table H-3 criteria or the correlation equation (where contaminant constants are available) is achievable by carbon in the PVP adsorption system.

Lastly, it is recognized that some contaminants will be extensively destroyed in the thermal oxidizer and will appear in the adsorption system at extremely dilute concentrations. These low concentrations may be considerably lower than the valid lower limit of either predictive method for capacity. To account for this uncertainty, the estimated adsorption DF of those compounds which show a high DF in the RTO will be reduced by a safety factor. It is assumed that a reduction factor of 10 for adsorption DFs on compounds which have an assigned DF of ≥ 50 in the RTO will adequately compensate for uncertainties in the predicted value based on low concentration. This assumption is incorporated in the analysis methodology (Section 4.4). However, since the combustion DFs have been assigned conservatively, it is recognized that some compounds may achieve a DF of greater than 50 in the RTO even though they have been assigned a lower DF. In these cases, or where the originating evolved contaminant concentrations are appreciably lower than 0.1 ppmv, it is possible that the conservatism of each assigned removal efficiency (adsorption DF) may no longer be conservatively bounding. While this may be the case for numerous identified (or unidentified) compounds, the effect of introduced error on predictions made using the estimated removal DFs will be insignificant. In those cases where the adsorption removal efficiencies may not be bounding due to low concentration, the effect on a mass balance or emissions estimate will be negligible.

5.6 Adsorption RE and DF relationship

As discussed in Section 3.6, removal of a contaminant from a gas stream via adsorption is dependant on the attraction between the contaminant and the adsorbent, the concentration of the contaminant, and the physical properties of the contaminant. These factors are used with empirical data to generate carbon loading capacities and adsorption isotherms. However, the generated (or calculated) isotherms are typically valid for gas phase concentrations above 0.1 or 1.0 ppmv. Extrapolations of equations or relationships which predict loading capacity or isotherm data to concentrations below 0.1 ppmv may become quite inexact. Historical process knowledge would suggest that pilot scale tests should be conducted to determine exact adsorption performance. This is impractical for the PVP adsorption system since wastes processed in PT contain numerous trace organic compounds and each waste has a different organic signature. Information from pilot testing of a single waste may not be applicable to a different waste source. Therefore, the relationship between removal efficiency and DF will be estimated on a more general basis by the following table.

Table H-4

Adsorption Capacity (g adsorbed/100 g carbon)	Removal Efficiency (RE) %	DF mass flow in / mass flow out
0	0	1
0.5	20	1.25
1	50	2
2	80	5
5	90	10
10	95	20
≥20	98	50

This relationship takes into account the conservatism which has been placed on the assignment of each adsorption capacity. Each assigned adsorption capacity has taken into account the potential for selective adsorption (replacement of a weakly attracted contaminant by a strongly attracted compound) and the potential for compounds to be present in much lower than reference concentrations (<0.1 ppmv).

The relationship between estimated adsorption capacity and DF is an enabling assumption. While every attempt has been made to add reasonable conservatism, the above DFs are only a generalized estimate. Any other more accurate means of assigning DFs would require both of two virtually non-attainable pieces of information: 1) the specific compounds and concentrations of adsorbable contaminants in the post oxidizer PVP system vent gas, and 2) the specific multi-component isotherm for each compound. Once the adsorption system is in service with offgas evolved from PT waste processing, it will be possible to take upstream and downstream samples and establish the extent to which this assumption is conservatively bounding.

6 Analysis

In order to handle data for the numerous compounds maintained in each of the separate lists, the computations were performed on Microsoft Excel spreadsheets. Example compounds are shown in the remainder of this section to illustrate how the compound physical property data and analysis methodology are used in the computations to assign the DFs. Trans-1,3-dichloropropene, ethylene dibromide, (compound numbers 7 and 14 from Table 1-1) and 1-heptanol (compound number 95 from Table 1-2), are examples which show the various considerations underpinning the assigned DF methodology.

6.1 Trans-1,3-Dichloropropene

The AIT of trans-1,3-dichloropropene is shown as 1130 °F (an estimated value; see source 29 at the end of Table 1-1). This value is subtracted from the operating temperature of the RTO (1600 °F) to establish the extent of destruction temperature above the AIT.

$1600 - 1130 = 470$ °F

The difference is then compared to the criteria of Table H-2. The difference of 470 °F is higher than 400 °F but not higher than 475 °F. The assigned destruction DE for this compound in the RTO is 98 % as

associated with compounds having AITs of at least 400 °F below the operating temperature. This value is shown in Table 2-1 of Attachment 2 (compound no. 7).

The DF is calculated using the DE of 98 % and Equation H-2 as follows:

$$DF = \frac{1}{\left(1 - \frac{98}{100}\right)} = 50$$

The DF is shown in Table 2-1 beside the DE value.

Next, the boiling point and molecular weight are compared with the criteria from Table H-3 to assign an adsorption capacity. Trans-1,3-dichloropropene shows a molecular weight of 111 g/mol and a normal boiling point of 112 °C. The uppermost row of Table H-3 for which this compound fits is the boiling range of 100 to 150 °C and molecular weight of <150. The estimated capacity is 2.0 g/100 g carbon. No quadratic constants for this compound are provided in the prediction correlation from Yaws 1995; therefore, the assigned capacity is 2.0 g/100 g carbon. This capacity is compared to the criteria from Table H-4, which shows the corresponding RE of 80 %. Equation H-2 applied to this RE gives a DF of 5. The adsorption RE and DF are shown in Table 3-1.

The final consideration for trans-1,3-dichloropropene is the potential for extremely low concentration in the feed gas to the adsorption process on behalf of extensive destruction in the RTO. Table 4-1 shows the assigned DFs for combustion and adsorption (see compound no. 7). Since the oxidizer DF is at least 50, the adsorption DF is reduced by a factor of 10. The reduced adsorption DF becomes 5/10 or 0.5 but the minimum DF as defined in Equation H-2 is 1.0. The reduced DF for trans-1,3-dichloropropene is shown as 1.0 in Table 4-1. This DF will result in a more conservative combined DF since credit is no longer being taken for removal via adsorption. The combined DF is:

oxidation DF x reduced adsorption DF = combined DF = 50 x 1 = 50 (as shown in Attachment 4, Table 4-1)

6.2 Ethylene Dibromide

The AIT of ethylene dibromide is shown as 1600 °F (an estimated value). According to the cited physical property source, the compound is considered nonflammable. Given that brominated methanes and ethanes (commonly classified as halons) are used as fire suppression agents and no other information was found available, the AIT value was assigned to be 1600 °F. This ensures that no credit for destruction will be taken in the RTO since the difference between AIT and operating temperature is zero. Criteria from Table H-2 shows that no credit for destruction is taken unless the operating temperature is at least 1.0 degree higher than the AIT. The corresponding DE is 0 % and so the DF has been assigned as 1.0 in accordance with Equation H-2. The DF is shown in Attachment 2, Table 2-1, beside the DE value (compound no. 14).

Next, the boiling point and molecular weight are compared with the criteria from Table H-3 to assign an adsorption capacity. Ethylene dibromide shows a molecular weight of ~188 g/mol and a normal boiling point of 131.7 °C. The uppermost row of Table H-3 for which this compound fits is the boiling range of 100 to 150 °C and molecular weight of at least 150. The corresponding estimated adsorption capacity is 5.0 g/100 g carbon.

Quadratic constants were found for using the capacity prediction correlation from Yaws 1995. The constants cited are:

A = 1.4423
B = 0.255
C= -0.0267

The predicted capacity by Equation H-3 is:

$$\log_{10} Q = A + B\log_{10} y + C[\log_{10} y]^2 = 1.4423 + 0.255\log_{10}(0.1) + (^{-}0.0267)[\log_{10}(0.1)]^2 = 1.16$$

$Q = 10^{1.16} = 14.5$ g ads/100 g carbon

This predicted value is higher than the estimated value using the graduated criteria from Table H-3, and so the estimated adsorption capacity of 5.0 (g /100 g carbon) is selected for this compound.

This capacity is compared to the criteria from Table H-4, which shows the corresponding RE of 90 %. Equation H-2 applied to this RE gives a DF of 10. The adsorption RE and DF are shown in Table 4-1.

The final consideration for ethylene dibromide is the potential for extremely low concentration in the feed gas to the adsorption process on behalf of extensive destruction in the RTO. Since no credit is taken for combustion of this compound, it does not have a destruction DF of 50 or higher. The combined DF and adsorption DF are the same for ethylene dibromide as shown in Table 4-1.

6.3 1-Heptanol

The AIT of 1-heptanol is shown as 320 °C (608 °F). This is a conservatively estimated value which is based on a referenced compound and the recognized trend of longer alkane chains associated with lower AITs (see source 34 at the end of Table 1-2). This value is subtracted from the operating temperature of the RTO (1600 °F) to establish the extent of combustion temperature above the AIT.

1600 – 608 = 992 °F

This difference is then compared to the criteria of Table H-2. The difference of 992 °F is higher than the maximum DE temperature criteria of 650 °F. The assigned destruction DE for this compound in the RTO is 99.99 % as associated with compounds having AITs of at least 650 °F below the operating temperature. This value is shown in Table 2-2 of Appendix 2 (compound no. 95).

The DF is calculated using the DE of 99.99 % and Equation H-2 as follows:

$$DF = \frac{1}{\left(1 - \frac{99.99}{100}\right)} = 10{,}000$$

The DF is shown in Table 2-2 beside the DE value.

Next, the boiling point and molecular weight are compared with the criteria from Table H-3 to assign an estimated adsorption capacity. 1-Heptanol shows a molecular weight of 116 g/mol and a normal boiling

point of 176 °C. The uppermost row of Table H-3 for which this compound fits is the boiling range of >150 °C and molecular weight of <150. The assigned capacity is 10.0 g/100 g carbon. This capacity is compared to the criteria from Table H-4, which shows the corresponding RE of 95 %. Equation H-2 applied to this RE gives a DF of 20. The adsorption RE and DF are shown in Table 3-2.

The final consideration for 1-heptanol is the potential for extremely low concentration in the feed gas to the adsorption process on behalf of extensive destruction in the RTO. Table 4-2 shows the assigned DFs for combustion and adsorption (see compound no. 95). Since the oxidizer DF for 1-heptanol (10,000) is at least 50, the adsorption DF is reduced by a factor of 10. The reduced adsorption DF becomes 20/10 or 2.0 as shown in Table 4-2.

Each of the compounds from Tables 1-1 and 1-2 are assigned DFs by the same methodology as these example compounds and are shown in Attachments 2, 3, and 4 in their respective tables.

7 Results and Conclusion

Results of this analysis as defined in the objective are shown in Tables 4-1 and 4-2 of Attachment 4. Without the correct identification of exact species and concentrations of organic contaminants in the PVP system offgas, a more sophisticated method for estimating adsorption performance cannot be used. For contaminants which may be present at less than measurable quantities in the adsorber feed gas, the extent of adsorption capacity may be significantly lower than what would be shown by criteria from Table H-3. However, at concentrations which may be relevant to environmental emissions estimates (near 0.1 ppmv), the analysis methodology can be considered conservative with respect to oxidation DFs. For adsorption DFs, every effort has been made to ensure that the methodology is reasonable and conservative. Pending the operational confirmation that criteria in Table H-4 is bounding behavior for the organic contaminants, the methodology for RE can be considered reasonable for contaminant concentrations near 0.1 ppmv.

The reduction of adsorption DF for use in calculating the combined DF of compounds with high DEs has been implemented to provide additional conservatism. Although the specific adsorption behavior of contaminants at ultra low concentrations is not known, the cumulative effect of compounds at trace quantities is negligible in terms of regulatory importance. As such, the assigned adsorption DFs from this analysis do not present any special requirements for the design of the adsorption system. The adsorption system can be considered complimentary to the oxidation abatement system as exemplified by ethylene dibromide (Section 6.2).

8 References

Project Documents

24590-WTP-RPT-ENS-03-006, Rev 0, *Environmental Risk Assessment Work Plan for the Hanford Tank Waste Treatment and Immobilization Plant.*

24590-PTF-3YD-PVP-00001, Rev 0, *System Description for Pretreatment Vessel Vent Process System, PVP.*

24590-PTF-M0C-PVP-00003, Rev B, *Sizing of Pretreatment Vessel Vent Carbon Adsorbers (PVP-ABS-00001A/B).*

Other Documents

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EPA-CICA. 1999. Environmental Protection Agency, *Air Pollution Technology Fact Sheet, Incinerator-Recuperative Type.*

Lewandowski, D. 2000. *Design of Thermal Oxidation Systems for Volatile Organic Compounds*, CRC Press LLC, Boca Raton, Florida.

Shepherd, A. 2001. Technology Paper: *Activated Carbon Adsorption for Treatment of VOC Emissions*, presented at the 13th EnviroExpo, Boston, Massachusetts, May 2001, Carbtrol Corporation, Bridgeport Connecticut.

Stock, L and Huckaby J. 2000. *A survey of Vapors in the Headspaces of Single-Shell Waste Tanks*, PNNL-13366, Pacific Northwest Nation Laboratory, Richland, WA. October 2000.

Wiemers, KD et al. 1998. *Regulatory Data Quality Objectives Supporting Tank Waste Remediation System Privatization Project*, PNNL-12040, Pacific Northwest National Laboratory, Richland, WA.

Yaws, C, Bu, L, and Nijhawan, S. 1995. *Determining VOC Adsorption Capacity,* Pollution Engineering. February 1995.

9 Attachments

Attachment	Content
Attachment 1	Tables of Contaminants and Physical Properties
Table 1-1	COPCs
Table 1-2	Compounds detected >0.1 ppmv
Attachment 2	Tables of Destruction DFs
Table 2-1	COPCs
Table 2-2	Compounds detected >0.1 ppmv
Attachment 3	Tables of Removal DFs
Table 3-1	COPCs
Table 3-2	Compounds detected >0.1 ppmv
Attachment 4	Tables of DF Analysis Results
Table 4-1	COPCs
Table 4-2	Compounds detected >0.1 ppmv
Attachment 5	Thermal Stability Ranking Study: Figure 9 of Technical Article *Development of a Thermal Stability Based Ranking of Hazardous Organic Compound Incinerability* (Dellinger 2000)
Attachment 6	VOC Properties and Adsorption Potential: Technology Paper *Activated Carbon Adsorption for Treatment of VOC Emissions* (Shepherd 2001)
Attachment 7	Prediction of VOC Adsorption Capacity: Technical Article *Determining VOC Adsorption Capacity* (Yaws 1995)

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Attachment 1 Tables of Contaminants and Physical Properties

Table 1-1 COPCs
Table 1-2 Compounds detected >0.1 ppmv

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Table 1-1 COPCs

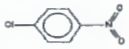
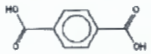
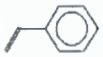
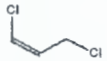
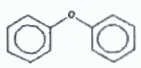
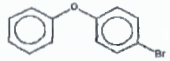
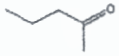
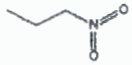
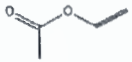
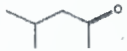
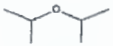
Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
 	1	100-00-5	p-Nitrochlorobenzene	157.56	C6H4ClNO2		242	0.01	510	950	47	
	2	100-21-0	p-Phthalic acid	166.13	C8H6O4	300	sublimes	0.6	677	1250	51	
	3	100-41-4	Ethyl benzene	106.16	C8H10		136.2	0.026	432	810	1	
	4	100-42-5	Styrene	104.14	C8H8		145.2	0.032	490	915	22	
	5	10061-01-5	cis-1,3-Dichloropropene	110.97	C3H4Cl2		104.3	0.1	600	1112	27	
	6	10061-02-6	trans-1,3-Dichloropropene	110.97	C3H4Cl2		112	0.1	610	1130	29	
 	7	101-55-3	4-Bromophenylphenyl ether	249.11	C12H9BrO		310.14	0.000001	839	1542.02	none	4
	8	101-84-8	Diphenyl ether	170.21	C12H10O	26.8	498	insoluble	618	1144	5	
	9	106-35-4	3-Heptanone	114.19	C7H14O		147	0.43	390	734	47	
	10	106-42-3	p-Xylene (Dimethyl benzene)	106.16	C8H10		138.3	0.02	530	986	1	
	11	106-46-7	1,4-Dichlorobenzene	147.01	C6H4Cl2	53.1	173.4	0.00813	640	1184	47	
	12	106-88-7	1,2-Epoxybutane	72.12	C4H8O		63.3	6	479	894.2	17	
	13	106-93-4	Ethylene dibromide (Dibromoethane)	187.88	C2H4Br2		131.7	0.41	871	1600	31	1
	14	106-97-8	Butane (R-600)	58.123	C4H10		-0.45	0.0061	405	761	1	
	15	106-99-0	1,3-Butadiene	54.091	C4H6		-4.4	0.05	449	840.2	22	
	16	107-02-8	Acrolein	56.06	C3H4O		52.7	21.25	235	455	1	
	17	107-05-1	3-Chloropropene (Allyl chloride)	76.526	C3H5Cl		44	0.337	485	905	1	
	18	107-06-2	1,2-Dichloroethane (Ethylene chloride) (freon 150	98.96	C2H4Cl2		83.5	0.86	412	773.6	1	
	19	107-12-0	Propionitrile	55.079	C3H5N		97.2	decomposes	510	950	7	
	20	107-13-1	Acrylonitrile	53.06	C3H3N		77.3	7.45	481	897.8	1	
	21	107-18-6	2-Propene-1-ol	58.08	C3H6O		97	32	378	712.4	1	
	22	107-31-3	Formic acid, methyl ester	60.05	C2H4O2		32	10	465	869	1	
	23	107-66-4	Dibutylphosphate	210.21	C8H19O4P		100	slightly	510	950	26	
	24	107-67-9	2-Pentanone	86.133	C5H10O		100	4.3	505	941	1	
	25	108-03-2	1-Nitropropane	89.09	C3H7NO2		131	1.4	420	788	1	
	26	108-05-4	Vinyl acetate	86.09	C4H6O2		72.3	2	427	800.6	1	
	27	108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	100.16	C6H12O		117.4	1.9	459	858	1	
	28	108-20-3	Bis(isopropyl)ether	102.18	C6H14O		68.5	0.2	443	829	9	
	29	108-38-3	m-Xylene (Dimethyl benzene)	106.16	C8H10		139.1	0.02	530	986	1	
	30	108-39-4	m-Cresol	108.13	C7H8O		202	1	559	1038.2	5	
	31	108-87-2	Methylcyclohexane	98.188	C7H14		101	insoluble	250	482	1	
	32	108-88-3	Toluene	92.13	C7H8		110.6	0.053	480	896	1	
	33	108-90-7	Chlorobenzene	112.56	C6H5Cl		130	0.05	674	1245	22	
	34	108-93-0	Cyclohexanol	100.16	C6H12O		161	3.6	300	572	5	
	35	108-94-1	Cyclohexanone	98.2	C6H10O		155.6	5	420	788	1	

Table 1-1 COPCs

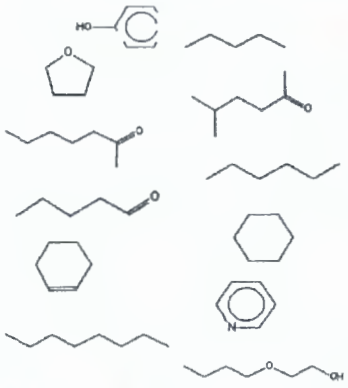
Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	36	108-95-2	Phenol	94.11	C6H6O		181.7	8.3	715	1319	21	
	37	109-66-0	n-Pentane	72.15	C5H12		36.1	0.04	260	500	1	
	38	109-99-9	Tetrahydrofuran	72.1	C4H8O		66	30	321	609.8	1	
	39	110-12-3	5-Methyl-2-hexanone	114.19	C7H14O		144	0.5	191	376	6	
	40	110-43-0	2-Heptanone	114.19	C7H14O		150	0.43	393	739	5	
	41	110-54-3	n-Hexane	86.177	C6H14		69	0.00095	225	437	1	
	42	110-62-3	n-Valeraldehyde	86.13	C5H10O		103	0.1	260	500	3	
	43	110-82-7	Cyclohexane	84.161	C6H12		80.7	0.1	245	473	1	
	44	110-83-8	Cyclohexene	82.145	C6H10		83	0.02	310	590	1	
	45	110-86-1	Pyridine	79.1	C5H5N		115.2	miscible	482	899.6	1	
	46	111-65-9	n-Octane	114.23	C8H18		126	slightly	220	428	1	
	47	111-76-2	Ethylene glycol monobutyl ether	118	C6H14O2		171	5	238	460.4	5	
straight chain C-9	48	111-84-2	n-Nonane	128.26	C9H20		150.8	0.1	190	374	1	
	49	117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	390.54	C24H38O4		386.9	0.000034	390	734	5	
	50	117-84-0	n-Dioctyl phthalate	390.56	C24H38O4		220	0.0003	391	735.08	55	
	51	120-12-7	Anthracene	178.22	C14H10		340	0.00000434	538	1000.4	55	
	52	120-82-1	1,2,4-Trichlorobenzene	181.46	C6H3Cl3		214.4	0.0049	571	1060	50	
	53	120-83-2	2,4-Dichlorophenol	163.01	C6H4Cl2O		210	0.45	839	1542.02	none	4
	54	121-44-8	Triethylamine	101.19	C6H15N		88.9	0.02	249	480	5	
	55	121-69-7	Dimethylaniline	121.18	C8H11N		194	1.6	371	699.8	5	
	56	122-39-4	N,N-Diphenylamine	169.23	C12H11N	52	302	0.03	634	1173	5	
	57	123-19-3	4-Heptanone	114.19	C7H14O		144	0.53	450	842	34	
	58	123-38-6	n-Propionaldehyde	58.08	C3H6O		49	5	207	404.6	1	
	59	123-51-3	3-Methyl-1-butanol	88.15	C5H12O		130	5.4	350	662	1	
	60	123-86-4	Acetic acid n-butyl ester	116.16	C6H12O2		126.1	0.68	425	797	1	
	61	123-91-1	1,4-Dioxane	88.1	C4H8O2		101.1	miscible	180	356	1	
	62	126-73-8	Tributyl phosphate	266.32	C12H27O4P		289	0.1	482	899.6	47	

Table 1-1 COPCs

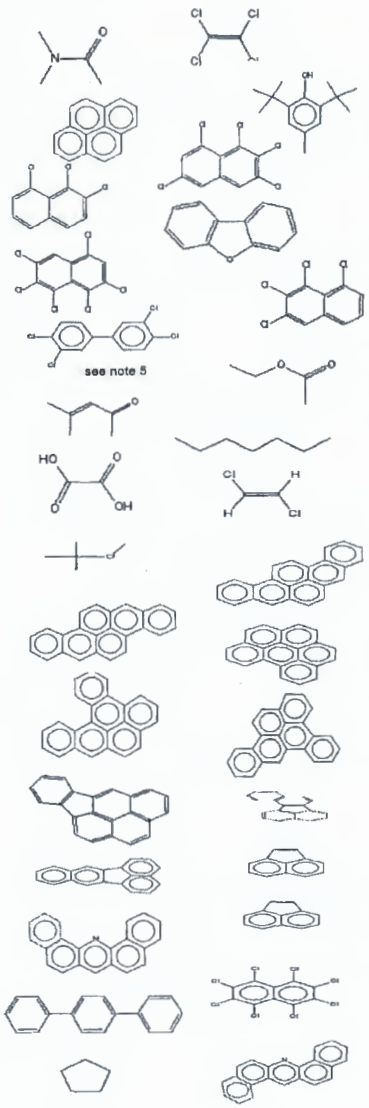
Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	63	126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	67.09	C4H5N		90.3	2.5	460	860	11	
	64	127-18-4	Perchloroethylene (tetrachloroethylene)	165.85	C2Cl4		121.1	0.015	871	1600	30	1
	65	127-19-5	N,N-Dimethylacetamide	87.12	C4H9NO		166	miscible	490	914	1	
	66	128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	220.35	C15H24O		265	insoluble	470	878	47	
	67	129-00-0	Pyrene	202.24	C16H10	156	404	0.0000013	839	1542.02	none	4
	68	1321-64-8	Pentachloronaphthalene	300.4	C10H3Cl5		327	insoluble	839	1542.02	none	4
	69	1321-65-9	Trichloronaphthalene	231.51	C10H5Cl3		304	insoluble	839	1542.02	none	4
	70	132-64-9	Dibenzofuran	168.19	C12H8O		285	0.1	839	1542.02	none	4
	71	1335-87-1	Hexachloronaphthalene	334.84	C10H2Cl6		343	insoluble	839	1542.02	none	4
	72	1335-88-2	Tetrachloronaphthalene	265.95	C10 H4 Cl4		316	insoluble	839	1542.02	none	4
see note 5	73	1336-36-3	Polychlorinated biphenyls (PCBs)	322	C12HxCly (x+y=10		>195	slightly	839	1542.02	none	4 & 5
	74	141-78-6	Acetic acid ethyl ester (Ethyl acetate)	88.1	C4H8O2		77.1	8	486	906.8	22	
	75	141-79-7	4-Methyl-3-penten-2-one	98.16	C6H10O		127	3	344	651	1	
	76	142-82-5	n-Heptane	100.2	C7H16		98.4	<0.01	223	433.4	1	
	77	144-62-7	Oxalic acid	90.035	C2H2O4		190	10	760	1400	39	
	78	156-60-5	trans-1,2-Dichloroethylene	96.95	C2H2Cl2		47.5	0.63	460	860	1	
	79	1634-04-4	Methyl tert-butyl ether	88.15	C5H12O		55.2	5.1	435	815	5	
	80	189-55-9	Dibenzo[a,i]pyrene	302.37	C24H14	308	404	0.0000013	839	1542.02	none	4
	81	189-64-0	Dibenzo[a,h]pyrene	302.37	C24H14	308	404	0.0000013	839	1542.02	none	4
	82	191-24-2	Benzo(g,h,i)perylene	276.34	C22H12		500	0.000000026	839	1542.02	none	4
	83	191-30-0	Benzo[a,l]pyrene	302.37	C24H14	162	404	0.0000013	839	1542.02	none	4
	84	192-65-4	Dibenzo[a,e]pyrene	302.37	C24H14	241	sublimes	0.0000013	839	1542.02	none	4
	85	193-39-5	Indeno(1,2,3-cd)pyrene	276.34	C22H12	162.5	536	0.0000062	839	1542.02	none	4
	86	206-44-0	Fluoranthene	202.26	C16H10	110.8	375	0.0000265	839	1542.02	none	4
	87	208-96-8	Acenaphthylene	152.21	C12H8	93.5	265	0.000393	839	1542.02	none	4
	88	2234-13-1	Octachloronaphthalene	403.73	C10Cl8	185	440	insoluble	839	1542.02	none	4
	89	224-42-0	Dibenz[a,j]acridine	279.34	C21H13N	216	>346	not found	839	1542.02	none	4
	90	226-36-8	Dibenz[a,h]acridine	279.34	C21H13N	228	>346	not found	839	1542.02	none	4

Table 1-1 COPCs

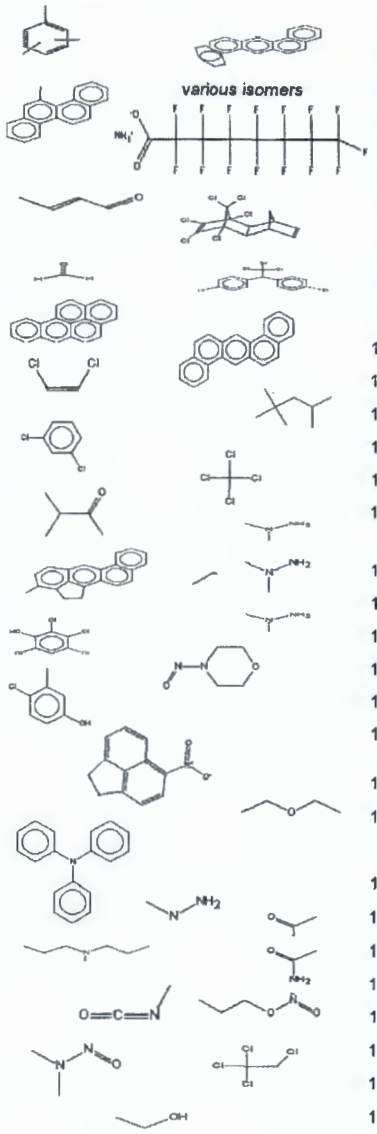
Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	91	25551-13-7	Trimethyl benzene	120.19	C9H12		164.7	insoluble	550	1022	1	
	92	26140-60-3	Terphenyls	230.31	C18H14	68	337	insoluble	839	1542.02	none	4
	93	27154-33-2	Trichlorofluoroethane	151.4	C2H2Cl3F		146.5	0.3	871	1600	36	2
	94	287-92-3	Cyclopentane	70.134	C5H10		49	insoluble	380	716	1	
	95	3697-24-3	5-Methylchrysene	242.32	C19H14	171	404	0.0000013	839	1542.02	none	4
	96	3825-26-1	Ammonium perfluorooctanoate	431.1	C8H4F15NO2	59	192	not found	839	1542.02	none	4
	97	4170-30-3	2-Butenaldehyde (2-Butenal)	70.091	C4H6O		102	18	230	446	16	
	98	50-00-0	Formaldehyde	30.03	CH2O		-19.5	55	430	806	1	
	99	50-32-8	Benzo(a)pyrene	252.3	C20H12	176.5	495	0.00000038	839	1542.02	none	4
	100	53-70-3	Dibenzo(a,h)anthracene	278.33	C22H14	266	524	0.00000005	839	1542.02	none	4
	101	540-59-0	1,2-Dichloroethylene	96.94	C2H2Cl2		48	0.5	460	860	21	
	102	540-84-1	2,2,4-Trimethylpentane	114.23	C8H18		99.2	insoluble	415	779	1	
	103	541-73-1	1,3-Dichlorobenzene	147.01	C6H4Cl2		173	0.0125	640	1184	47	
	104	56-23-5	Carbon tetrachloride (R-10)	153.84	CCl4		76.7	0.0805	871	1600	8	1
	105	563-80-4	3-Methyl-2-butanone	86.133	C5H10O		94	slightly	452	845.6	6	
	106	56-49-5	3-Methylcholanthrene	268.36	C21H16	179	280	0.0000013	839	1542.02	none	4
	107	57-14-7	1,1-Dimethylhydrazine	60.099	C2H8N2		63	decomposes	249	480.2	1	
	108	58-90-2	2,3,4,6-Tetrachlorophenol	231.9	C6H2Cl4O	70	150	slightly	839	1542.02	none	4
	109	591-78-6	2-Hexanone	100.16	C6H12O		127	1.4	533	991	1	
	110	59-50-7	4-Chloro-3-methylphenol	142.58	C7H7ClO	67	235	0.385	839	1542.02	none	4
	111	59-89-2	N-Nitrosomorpholine	116.12	C4H8N2O2	29	224	10	500	932	40	
	112	602-87-9	5-Nitroacenaphthene	199.21	C12H9NO2	102	279	0.1	839	1542.02	none	4
	113	60-29-7	Ethyl ether	74.12	C4H10O		34.6	6.9	160	320	1	
	114	603-34-9	Triphenylamine	245.32	C18H15N	127	347	0.1	839	1542.02	none	4
	115	60-34-4	Methylhydrazine	46.072	CH6N2		87.8	0.1	196	384.8	1	
	116	60-35-5	Acetamide	59.07	C2H5NO		221	10	480	896	15	
	117	621-64-7	Di-n-Propylnitrosamine	130.19	C6H14N2O		206	0.9894	275	527	43	
	118	624-83-9	Methyl isocyanate	57.052	C2H3NO		39	decomposes	535	995	13	
	119	627-13-4	Nitric acid, propyl ester	105.09	C3H7NO3		110	insoluble	420	788	28	
	120	62-75-9	N-Nitroso-N,N-dimethylamine	74.1	C2H6N2O		153	10	500	932	37	
	121	630-20-6	1,1,1,2-Tetrachloroethane	167.85	C2H2Cl4		130.5	0.1	871	1600	24	1
	122	64-17-5	Ethyl alcohol	46.069	C2H6O		78.3	10	426	798.8	22	

Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	123	64-18-6	Formic acid	46.03	CH2O2		100.7	miscible	434	813.2	1	
	124	64-19-7	Acetic acid	60.052	C2H4O2		118	miscible	465	869	1	
	125	67-56-1	Methyl alcohol (Methanol)	32.04	CH4O		64.6	miscible	470	878	1	
	126	67-63-0	2-Propyl alcohol (Isopropanol)	60.096	C3H8O		82.4	miscible	456	852.8	1	
	127	67-64-1	2-Propanone (Acetone)	58.08	C3H6O		56.2	miscible	465	869	1	
	128	67-66-3	Chloroform (R-20)	119.39	CHCl3		61.7	0.795	1000	1832	6	
	129	67-72-1	Hexachloroethane	236.74	C2Cl6	187	sublimes	0.005	871	1600	none	4
	130	684-16-2	Hexafluoroacetone	166.02	C3F6O		-26	miscible/reacts	871	1600	23	1
	131	71-23-8	n-Propyl alcohol	60.096	C3H8O		97.2	miscible	440	824	1	
	132	71-36-3	n-Butyl alcohol	74.1	C4H10O		117.6	6.32	367	692.6	22	
	133	71-43-2	Benzene	78.11	C6H6		80.1	0.18	592	1097.6	22	
	134	71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	133.42	C2H3Cl3		74.1	0.1495	537	999	9	
	135	74-83-9	Bromomethane (Methyl bromide) (halon 1001)	94.95	CH3Br		3.56	1.5	537	998.6	9	
	136	74-87-3	Chloromethane (Methyl chloride) (R-40)	50.49	CH3Cl		-24.2	0.533	662	1223.6	22	
	137	74-97-5	Bromochloromethane (halon 1011)	129.39	CH2BrCl		67.8	0.1	871	1600	24	1
	138	74-99-7	Methylacetylene	40.07	C3H4		-23	not found	340	644	12	
	139	75-00-3	Chloroethane	64.52	C2H5Cl		12.3	0.574	519	966.2	8	
	140	75-01-4	Vinyl chloride (1-Chloroethene)	62.5	C2H3Cl		-13.9	0.11	472	881.6	9	
	141	75-05-8	Acetonitrile	41.05	C2H3N		81.6	miscible	524	975.2	1	
	142	75-07-0	Acetaldehyde	44.05	C2H4O		20.1	miscible	175	347	1	
	143	75-09-2	Dichloromethane (Methylene chloride) (R-30)	84.94	CH2Cl2		39.8	1.32	662	1223.6	58	
	144	75-12-7	Formamide	45.04	CH3NO		210	miscible	500	932	4	
	145	75-15-0	Carbon disulfide	76.14	CS2		46.2	0.12	125	257	1	
	146	75-21-8	Ethylene oxide (Oxirane)	44.05	C2H4O		10.7	miscible	429	804.2	1	
	147	75-27-4	Bromodichloromethane	163.83	CHBrCl2		90.1	0.674	871	1600	none	3
	148	75-34-3	1,1-Dichloroethane	98.97	C2H4Cl2		57.3	0.51	456	852.8	1	
	149	75-35-4	1,1-Dichloroethene (Vinylidene chloride)	96.95	C2H2Cl2		31.7	0.23	457	854.6	9	
	150	75-43-4	Dichlorofluoromethane (R-21)	102.92	CHCl2F		9	insoluble	552	1026	56	2
	151	75-45-6	Chlorodifluoromethane (R-22)	86.47	CHClF2		-40.8	0.3	632	1170	9	
	152	75-50-3	Trimethylamine	59.11	C3H9N		2.87	miscible	190	374	6	
	153	75-52-5	Nitromethane	61.04	CH3NO2		101	9.5	418	784.4	1	
	154	75-55-8	2-Methylaziridine	57.1	C3H7N		66	miscible	490	914	14	
	155	75-61-6	Difluorodibromomethane (freon 12B2- halon 120	209.82	CBr2F2		24	0.1	871	1600	9	2
	156	75-63-8	Trifluorobromomethane (R-13B1)	148.91	CBrF3		-57.8	0.03	871	1600	9	1
	157	75-65-0	2-Methyl-2-propanol	74.122	C4H10O		82.2	miscible	478	892.4	5	

Table 1-1 COPCs

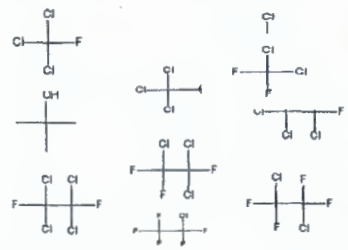
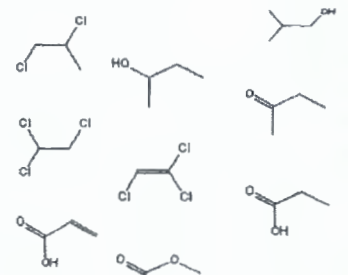
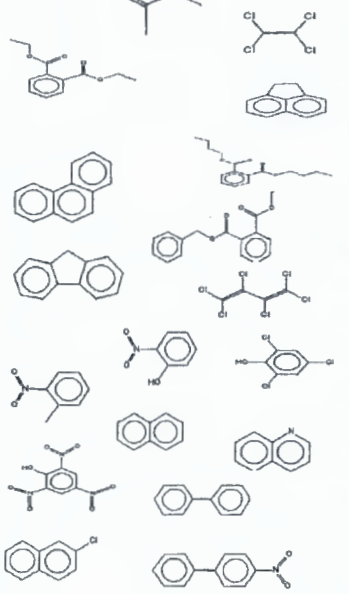
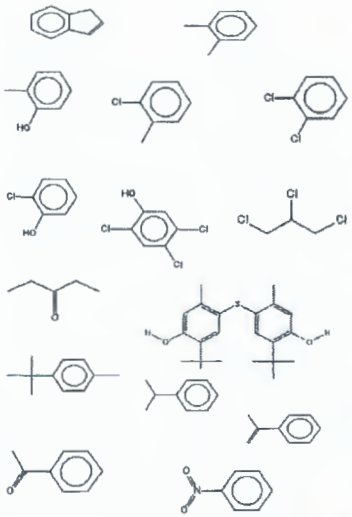
Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	158	75-69-4	Trichlorofluoromethane (R-11)	137.38	CCl3F		23.8	0.124	871	1600	8	2
	159	75-71-8	Dichlorodifluoromethane (R-12)	120.92	CCl2F2		-29.79	0.03	871	1600	9	2
	160	76-03-9	Trichloroacetic acid	163.39	C2HCl3O2	57	196	10	871	1600	5	2
	161	76-11-9	1,1,1,2-Tetrachloro-2,2-difluoroethane (R-112a)	203.83	C2Cl4F2	41	91	0.01	732	1350	25	
	162	76-12-0	1,1,2,2-Tetrachloro-1,2-difluoroethane (R-112)	203.83	C2Cl4F2	26	93	0.01	732	1350	25	
	163	76-13-1	1,2,2-Trichloro-1,1,2-trifluoroethane (Freon 113)	187.38	C2Cl3F3		47.6	0.02	680	1256	9	
	164	76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane (R-114)	170.92	C2Cl2F4		3.8	slightly	871	1600	9	2
	165	76-15-3	Chloropentafluoroethane (R-115)	154.47	C2ClF5		-39.1	insoluble	871	1600	9	2
	166	78-83-1	2-Methylpropyl alcohol (Isobutyl alcohol)	74.12	C4H10O		107.9	9.5	415	779	9	
	167	78-87-5	1,2-Dichloropropane	112.99	C3H6Cl2		96.8	0.27	557	1034	1	
	168	78-92-2	1-Methylpropyl alcohol (2-Butanol)	74.122	C4H10O		99.5	15	406	762.8	1	
	169	78-93-3	Methyl ethyl ketone (MEK, 2-Butanone)	72.1	C4H8O		79.6	25.6	516	960.8	2	
	170	79-00-5	1,1,2-Trichloroethane	133.42	C2H3Cl3		113.8	0.442	500	932	22	2
	171	79-01-6	Trichloroethylene	131.4	C2HCl3		86.7	0.11	420	788	5	
	172	79-09-4	Propionic acid	74.08	C3H6O2		140.7	37	490	914	18	
	173	79-10-7	2-Propenoic acid	72.06	C3H4O2	12	141.6	10	438	820.4	5	
	174	79-20-9	Methyl acetate	74.08	C3H6O2		56.9	24.5	502	935.6	1	
	175	79-34-5	1,1,2,2-Tetrachloroethane	167.86	C2H2Cl4		146.3	0.3	871	1600	9	2
	176	83-32-9	Acenaphthene	154.21	C12H10	95	279	0.00035	839	1542.02	none	4
	177	84-66-2	Diethyl phthalate	222.24	C12H14O4		298	0.09	457	855	5	
	178	84-74-2	Dibutyl phthalate	278.34	C16H22O4		340	0.0013	402	756	5	
	179	85-01-8	Phenanthrene	178.22	C14H10	99.5	340	0.00012	839	1542.02	none	4
	180	85-68-7	Butylbenzyl phthalate	312.39	C19H20O4		370	0.00027	233	451.4	52	
	181	86-73-7	Fluorene	166.22	C13H10	116	295	0.000019	839	1542.02	none	4
	182	87-68-3	Hexachlorobutadiene	260.76	C4Cl6		210	0.00032	610	1130	55	
	183	88-06-2	2,4,6-Trichlorophenol	197.46	C6H3Cl3O	69.5	244.5	0.08	839	1542.02	none	4
	184	88-72-2	2-Nitrotoluene	137.13	C7H7NO2		221	0.06	305	581	44	
	185	88-75-5	2-Nitrophenol	139.11	C6H5NO3	45.3	214.6	0.21	839	1542.02	none	4
	186	88-89-1	Picric acid	229.11	C6H3N3O7	122	>300	1.4	300	572	none	
	187	91-20-3	Naphthalene	128.16	C10H8	80.6	218	0.00031	568	1054	1	
	188	91-22-5	Quinoline	129.16	C9H7N		238	0.01	480	896	5	
	189	91-58-7	2-Chloronapthalene	162.61	C10H7Cl	59.5	256	0.000674	839	1542.02	none	4
	190	92-52-4	1,1'-Biphenyl	154.21	C12H10	70	255	insoluble	540	1004	55	

Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		
	191	92-93-3	4-Nitrobiphenyl	199.21	C12H9NO2	113.8	340	insoluble	839	1542.02	none	4
	192	95-13-6	Indene	116.16	C9H8	58	181.6	insoluble	526	979	41	
	193	95-47-6	o-Xylene	106.16	C8H10		144	0.017	465	869	1	
	194	95-48-7	o-Cresol (2-Methylphenol)	108.13	C7H8O	30.9	191	0.1	559	1038.2	5	
	195	95-49-8	2-Chlorotoluene	126.59	C7H7Cl		159	slightly	500	932	37	
	196	95-50-1	o-Dichlorobenzene (1,2-Dichlorobenzene)	147.01	C6H4Cl2		180.5	0.0084	640	1184	47	
	197	95-57-8	2-Chlorophenol	128.56	C6H5ClO	7	175.6	2.85	415	779	53	
	198	95-95-4	2,4,5-Trichlorophenol	197.46	C6H3Cl3O	68	253	0.12	839	1542.02	none	4
	199	96-18-4	1,2,3-Trichloropropane	147.43	C3H5Cl3		156	0.18	500	932	37	
	200	96-22-0	3-Pentanone	86.133	C5H10O		101	4.7	450	842	1	
	201	96-69-5	Bis(3-tert-butyl-4-hydroxy-6-methyl-phenyl)sulfide	358.54	C22H30O2S	150	316	<0.01	839	1542.02	none	4
	202	98-51-1	p-tert-Butyltoluene	148.25	C11H16		193	<0.1	510	950	47	
	203	98-82-8	Cumene	120.19	C9H12		151	0.005	424	795	1	
	204	98-83-9	alpha-Methylstyrene	118.18	C9H10		165.4	<0.1	574	1065.2	42	
	205	98-86-2	Acetophenone	120.5	C8H8O	19.6	201.7	0.55	571	1059.8	5	
	206	98-95-3	Nitrobenzene	123.11	C6H5NO2	5.7	210.8	0.19	482	899.6		

Notes:
General- Boiling points were taken from Chemfinder (http://chemfinder.cambridgesoft.com) or NIST (http://webbook.nist.gov/chemistry/) where lowest value is not found with the AIT source.
1- MSDS shows compound is non flammable. AIT shown is reported as 1600 deg F to ensure that minimal credit is taken for removal efficiency through thermal oxidizer.
2- MSDS shows no AIT information and reports neglible fire hazard. AIT shown is 1600 deg F for same reason as note 1.
3- No MSDS or AIT information can be found for this compound. Due to its single carbon and 3 halogen structure, it will be treated similar to chloroform.
4- compounds with normal boiling points above 200, contain aromatic rings, and contain numerous halogen substitutions are treated as PCB in terms of AIT - in cases where no AIT information could be found - an AIT of 1542 will be used in this case in accordance with TSCA guidlines for destruction of PCBs of 2192 deg F, 2 sec res time, and 3% excess air in combustion products (this is a back calculated AIT from the efficiency predicted in table 3-2 of Lewandowski - Design on Thermal Oxidation Systems. This will be used for non halogenated napthalenic compounds as well in order to be conservative (pyrene, perlene etc).
5- structure shown is 1-1'-biphenyl,3,3',4,4'-tetrachloro (CAS# 32598-13-3) and is shown under the general context of PCBs to present a typical structure for chlorine substitutions on the biphenyl structure. Numerous variations of chlorine substitutions exist with the broad group of PCBs, however within this calculation, the treatment of PCBs under one set of compound properties is appropriate since the important properties do not range across DF boundary threshold values.
6- All BHC compound structures are the same except for the cis/trans orientation of the chlorine substitutions. (see Alpha BHC - CAS#319-84-6)
7- Camphene is the root structure of toxaphene which has 8 chlorine substitutions - no structure was found for toxaphene

Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		

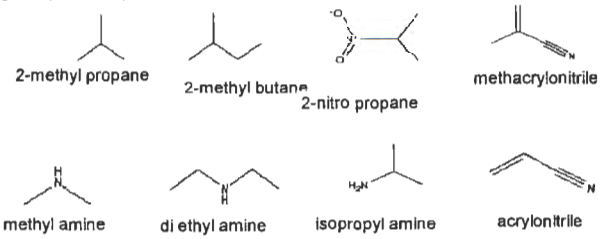
AIT Sources

1 Lange's Handbook of Chemistry - 14th edition
2 MSDS - EXXON CHEMICAL AMERICAS DIV. (http://www.temarry.com/MSDS/Methyl_Ethyl_Ketone_msds.htm)
3 n-Valeraldehyde is a synonym for pentanal. The AIT is estimated from the sequence of increasing carbon aldehydes: acetaldehyde (ethanal)-175 deg C, propionaldehyde (propanal)-207 deg C, butanal-230 deg C.
4 MSDS from Internation Programme on Chemical Safety (http://www.ilo.org/public/english/protection/safework/cis/products/icsc/dtasht/_icsc08/icsc0891.pdf)
5 MSDS from JT Baker (http://www.jtbaker.com/msds/a0120.htm)
6 MSDS (http://www.bandj.com/MainWindowPages/MSDS/DimAcetaMSDS.htm#5)
7 estimated from MSDS of acetonitrile - precision pure solvents (http://www.purificationtech.com/techacmsds3.htm)-524 deg C and safety data of butyronitrile from Physical and Theoretical Chemistry Lab (http://physchem.ox.ac.uk/MSDS/BU/butyronitrile.html)-488 deg C.
8 MSDS - BOC Gases (http://www.vngas.com/pdf/g32.pdf)

9 MSDS - MATHESON TRI-GAS, INC (http://www.matheson-trigas.com/mathportal/msds/)

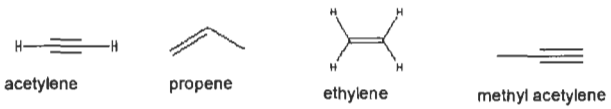
10 estimated from Langes Handbook of chemistry for 1,1-dichloroethylene - (570 deg C) instead of cis-1,2-dichloroethylene - (460 deg C)
11 AIT is estimated by comparison with the following compounds: (see structures to the right)

2-methyl propane - 462 deg C (source #1)
2-methyl butane - 420 deg C (source #9)
2-nitropropane - 428 deg C (source #1)
dimethylamine - 400 deg C (source #1)
diethylamine - 312 deg C (source #1)
acrylonitrile - 481 deg C (source #1)
isopropyl amine - 402 deg C (source #1)



12 AIT is estimated by comparison with the following compounds: (see structures to the right)

acetylene - 305 deg C (source # 1)
propene - 460 deg C (source # 1)
ethylene - 490 deg C (source # 1)



13 University of Akron Hazardous Chemical Database (http://ull.chemistry.uakron.edu/erd/)
14 AIT is estimated by comparison with the following compounds: (see structures to the right)

pyrrolidine - 345 deg C (source: BASF MSDS (http://www.basf.com/businesses/chemicals/pdfs/pyrrdine.pdf)
tetrahydrofuran - 321 deg C (source # 1)
propylene oxide - 449 deg C (source # 1)

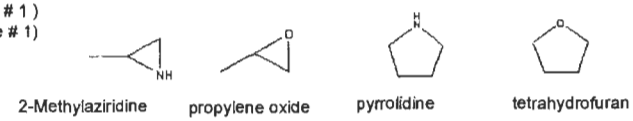
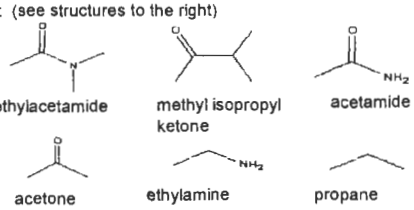


Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		

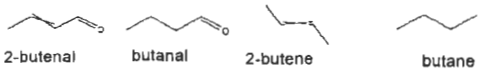
15 AIT is estimated by comparison with the following compounds: (see structures to the right)

ethylamine - 385 deg C (source: #1)
propane - 450 deg C (source # 1)
acetone - 465 deg C (source # 1)
dimethylacetamide - 490 deg C (source #1)
methyl isopropyl ketone - 452 deg C (source #6)



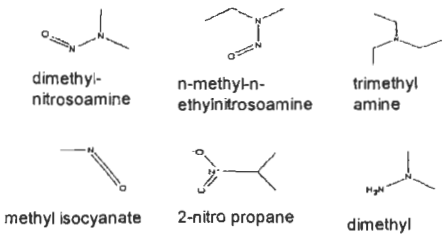
16 AIT is estimated by comparison with the following compounds: (see structures to the right)

butanal - 230 deg C (source #1)
butane - 405 deg C (source #1)
2-butene - 324 deg C (source #1)



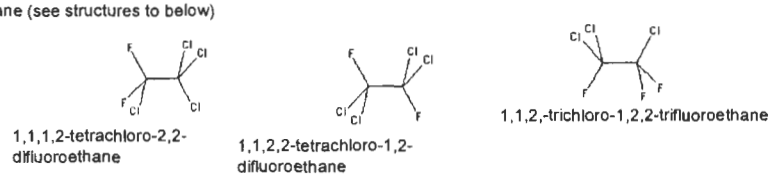
17 AIT is estimated from ethylene oxide (429 deg C) and propylene oxide (449 deg C) (CAS# 's 75-21-6 and 75-56-9 from AIT source #1)
18 AIT is estimated from formic acid (434 deg C) and acetic acid (465 deg C) CAS#'s 64-18-6 and 64-19-7 from AIT source #1
19 AIT is estimated by comparison with the following compounds: (see structures to the right)

trimethyl amine - 249 deg C (source #1)
methyl isocyanate - 535 deg C (source #1)
2-nitropropane - 428 deg C (source #1)
dimethyl hydrazine - 249 deg C (source #1)



20 sigma chemical MSDS (http://msds.pdc.cornell.edu/msds/siri/msds/h/q427/q266.html)
21 occupational safety and health guideline for phenol (http://www.osha-slc.gov/SLTC/healthguidelines/phenol/)
22 "Optimized Design and Operating Parameters for Minimizing Emissions During VOC Thermal Oxidation", Edward Donley and David Lewandowski. 88th Annual Meeting of Air & Waste Mgmt Assoc., 1995
23 MSDS from P & M Scientific Industrial Assoc (http://www.fluorine.ru/products/msds/others/hexafluoroacetone_msds.html)
24 International Chemical safety cards (http://hazard.com/msds/mf/cards/list.html)
25 AIT is estimated from 1,1,2-trichloro-1,2,2-trifluoroethane (see structures to below)

1,1,2,-trichloro-1,2,2-trifluoroethane - 680 deg C
1,1,1,2-tetrachloro-2,2-difluoroethane - 732 deg C
1,1,2,2-tetrachloro-1,2-difluoroethane - 732 deg C

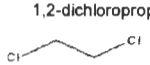


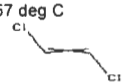
26 MSDS from OxyChem (http://new.www.oxychem.com/products/msds/m7623.pdf)
27 estimated from 1,2-dichloropropane (AIT is 557 deg C from source 1)

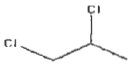
Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		

28 estimated from 1-nitropropane (AIT is 420 deg C from source 1)
29 AIT is estimated from 1,2 dichloropropane (see structures to below)
1,2-dichloroethane - 412 deg C
1,2-dichloroethylene - 460 deg C
1,2-dichloropropane - 557 deg C


1,2-dichloroethane


1,2-dichloroethylene

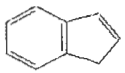

1,2-dichloropropane

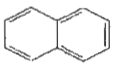
1,3-dichloropropene

30 Hill Brothers Chemical Co. MSDS (http://hillbrothers.com/msds/perchloro.htm)
31 OCCUPATIONAL SAFETY AND HEALTH GUIDELINE FOR ETHYLENE DIBROMIDE (http://www.osha-slc.gov/SLTC/healthguidelines/ethylenedibromide/recognition.html#healthhazard)
32 OCCUPATIONAL SAFETY AND HEALTH GUIDELINE FOR HEPTACHLOR (http://www.osha-slc.gov/SLTC/healthguidelines/heptachlor/)
33 Albaugh, INC. MSDS (http://www.cdms.net/idat/mp4JE001.pdf)
34 AIT estimated from 2-heptanone - 393 deg C (source #5)
35 No AIT information was found available. Because this molecule has multiple unsaturated bonds and chlorine attachments, its AIT is estimated at 1542 deg F. This temperature fits the prediction table by back calculation when using TSCA guidelines on incineration of PCBs at minimum temperatures of 2192 deg F for achieving 99.99% destruction.

36 AIT is estimated by comparison with tetrachloroethanes from above (CAS#'s 630-20-6 and 79-34-5)
37 AIT is Conservatively estimated at 500 deg C since MSDS has no stated AIT but uses NFPA fire rating of 2 - compound is therefore assumed flammable at a reasonable AIT

38 AIT is estimated from N-Nitroso-N,N-dimethylamine (CAS# 62-75-9)
39 Compound is shown to decompose at high temperatures. AIT is estimated at 1400 deg F to be conservative
40 Compound is conservatively estimated to have AIT of less than 500 deg C based on its lack of halogens and double bonds (resonance stabilized structure)
41 AIT is estimated by Napthalene (see structures below)


indene


naphthalene

42 AMS MSDS (http://www.kpb.co.kr/eng/product/msds_AMS.htm)
43 Chemical Land 21.com Phys and Chem properties (http://www.chemicalland21.com/arokorhl/industrialchem/organic/DIPROPYLAMINE.htm)
44 Physical and Theoretical Chemistry Laboratory - Oxford University (http://physchem.ox.ac.uk/MSDS/)
45 AIT is conservatively estimated at 1600 deg F by comparison to Phenol with additional chlorine substitutions
46 AIT is conservatively estimated from Trans-1,3-dichloropropene (610 deg C) and 1,2 dichloropropane (557 deg C)
47 MSDS - Fisher Scientific Canada (http://www.fishersci.ca/homepage2.nsf/frmSearch?CreateDocument&lang=E&AID=waSearch&DB=msds.nsf) or by link at (http://www-woc.sci.kun.nl/cgi-bin/view?xylenol)
48 occupational safety and health guideline (http://www.osha-slc.gov/SLTC/healthguidelines)
49 No AIT information was found available - AIT is conservatively estimated at 1600 deg F since compound has multiple halogen substitutions
50 MSDS - Baxter Healthcare Burdick & Jackson Div. (http://www-woc.sci.kun.nl/cgi-bin/view?xylenol)
51 MSDS - Amoco (http://www-woc.sci.kun.nl/cgi-bin/view?xylenol)
52 MSDS from NPS chemical repository (http://ntp-support.niehs.nih.gov/ntp_reports/ntp_chem_h&s/ntp_chem8/radian85-68-7.txt)
53 AIT is estimated from 4-chlorophenol which is listed in source 5
54 AIT is estimated from 1-chloro-4-nitrobenzene (CAS# 100-00-5)
55 MSDS - NTP chemical repository (http://157.98.10.135/NTP_Reports/NTP_Chem_H&S/NTP_Chem1/Radian117-84-0.txt)
56 Chemical Properties Handbook, C. L. Yaws, 1999 McGraw-Hill Publishing

Table 1-1 COPCs

Structure	no. of compound	CAS #	COPCs	MW	formula	melting point (if above 0°C)	normal boiling point	water solubility	AIT	AIT	AIT source	Compound information Note
			Compound	g/mol		°C	°C	g/100mL	deg C	deg F		

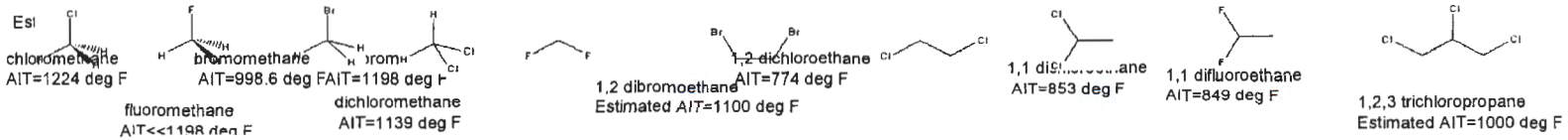
57 estimated from the following sources and structural comparison:

Sources:
* 1,1 difluoroethane AIT of 849 deg F - from Dupont chemical MSDS (http://www.dupont.com/msds/40_37_3027fr.html)
* difluoromethane AIT of 986 deg F - from Mational Industrial Chemicals Notification and assessment Scheme Report: (http://www.nicnas.gov.au/publications/CAR/new/NA/NAFULLR/NA0500FR/NA563FR.pdf)
* No AIT for flouromethane could be found - however, the NFPA flammability rating for this compound is 4 and the AIT is assumed to be much less than difluoromethane.

*1,2 dichloromethane AIT of 1186 deg F is listed above
*chloromethane AIT of 1224 deg F is listed above
*1,2 dichloroethane AIT of 774 deg F is listed above
*1,1 dichloroethane AIT of 853 deg F is from Langes Handbook (source 1 from above)
* 1,2,3 trichloropropane AIT of 580 deg F - from NTP chemical repository MSDS: (http://ntp-server.niehs.nih.gov/htdocs/Chem_H&S/NTP_Chem9/Radian96-18-4.html)

*bromomethane AIT of 998.6 deg F is listed above

Est



58 University of Akron - Chemical Database (http://ull.chemistry.uakron.edu/erd/)

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
none	1	Cyclotrisiloxane, hexamethyl-	222.5	541-05-9	C6H18O3Si3	65	134	"moisture sensitive"	1	400	53		
	2	Cyclotetrasiloxane, octamethyl-	296.6	556-67-2	C8H24O4Si4	17.5	175	"insoluble"	6	400	42	2	typically found in adhesives and sealant materials
	3	tetramethylcyclotrisiloxane	194.0	USI000-06	C4H14O3Si3	-65	135	"insoluble"	3	250	2	3	made for tetramethylcyclotetrasiloxane - also shows reactive with water
	4	Benzenesulfonamide, N-butyl-	213.3	3622-84-2	C10H15NO2S		314	practically insoluble"	2	800	54	1	
	5	2(3H)-Furanone, dihydro-3,5-dimethyl-	114.1	5145-07-1	C6H10O2	-31	206	"completely"	4	425	13		
	6	Pyridine, 2,4-dimethyl-	107.2	108-47-4	C7H9N	-60	159		5	482	3		
	7	Furan, tetrahydro-	72.1	109-99-9	C4H8O		66	<0.1	1	321	1		
	8	Furan	68.1	110-00-9	C4H4O	-85.6	31.4	<0.1	1	360	42		
	9	Pyridine	79.1	110-86-1	C5H5N	-41.6	115.2	"miscible"	1	482	1		
	10	Furan, 2,5-dihydro-	70.1	1708-29-8	C4H6O		67		5	450	10		
	11	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, tra	128.2	24405-16-1	C7H12O2		180		7	350	12		
	12	Pyrimidine	80.1	289-95-2	C4H4N2	20	123		1	450	11		
	13	Pyrazine	80.1	290-37-9	C4H4N2	52	115		1	450	11		
	14	Furan, 2-methyl-	82.1	534-22-5	C5H6O	-88.7	63	<0.1	1	450	10		
	15	Oxirane, ethenyl-	70.1	930-22-3	C4H6O	-85.7	67	1-5	5	429	14		
	16	2(3H)-Furanone, dihydro- (gamma butyrolact	86.1	96-48-0	C4H6O2	-43	205	10	5	450	10		
	17	1,3-Propanediol, dinitrate	166.1	3457-90-7	C3H6N2O6		100		7	450	9		boiling pt estimated by nitric acid propyl ester
	18	1,4-Butanediol, dinitrate	180.1	3457-91-8	C4H8N2O6	12	130		5*	450	9		boiling pt estimated by nitric acid butyl ester
	19	Nitrous acid, butyl ester	103.1	544-16-1	C4H9NO2		78		5	450	7	3	
	20	Nitrous acid, methyl ester	61.0	624-91-9	CH3NO2	-83	64.6		6	500	6		
	21	Nitric acid, ethyl ester	91.1	625-58-1	C2H5NO3	-102	88	"decomposes"	5	90	1		
	22	Butane, 1-nitro-	103.1	627-05-4	C4H9NO2	-81	153	slightly	5	450	4		
	23	Nitric acid, propyl ester	105.1	627-13-4	C3H7NO3	-100	110	"insoluble"	1	175	1		reported as "insoluble"
	24	Methanamine, N-methyl-N-nitroso- and other	74.1	62-75-9	C2H6N2O		153		5	500	17		
	25	Nitric acid, butyl ester	119.1	928-45-0	C4H9NO3		136		5	400	5		
	26	Pyrrolidine	71.1	123-75-1	C4H9N	-61	87		5	450	6		
	27	Methanamine, N-(1-methylbutylidene)-	99.2	22431-09-0	C6H13N		130		7	350	16		boiling pt estimated from hexamethyleneimine
	28	2-Pyrrolidinone	85.1	616-45-5	C4H7NO	24	245		1	450	15		
	29	Methanamine, N,N-dimethyl-	59.1	75-50-3	C3H9N	-117	2.9	miscible	1	190	1		
	30	Propanenitrile	55.1	107-12-0	C3H5N	-93	97	5-10	5	510	17		reported to decompose in aqueous solution
	31	Butanenitrile	69.1	109-74-0	C4H7N	-112	118	slightly	1	488	18		
	32	Pentanenitrile	83.1	110-59-8	C5H9N	-96	139	0.1-0.5	1	475	19		
similar to above	33	Octanenitrile	125.2	124-12-9	C8H15N	-45	199		1	450	19		
similar to above	34	Nonanenitrile	139.2	2243-27-8	C9H17N	-35	224		1	440	19		
similar to above	35	Hexanenitrile	97.2	628-73-9	C6H11N	-80	162		5	470	19		
similar to above	36	Heptanenitrile	111.2	629-08-3	C7H13N	-63	180		5	460	19		
	37	Acetonitrile	41.1	75-05-8	C2H3N	-48	81	miscible	1	524	1		
	38	Butanoic acid, butyl ester	144.2	109-21-7	C8H16O2	-92	166		1	450	20		
	39	Tetradecanoic acid, 1-methylethyl ester	270.5	110-27-0	C17H27O2		300		1*	400	21		boiling pt estimated from Pentadecanoic acid
	40	Butanedioic acid, diethyl ester	174.2	123-25-1	C8H14O4	-20	217		1	350	24	1	
	41	Acetic acid, butyl ester	116.2	123-86-4	C6H12O2	-106	126	0.68	1	425	1		
	42	Phosphoric acid tributyl ester	266.3	126-73-8	C12H27O4P	-80	289	0.1	1	482	17		

Table 1-2 Compounds detected > 0.1 ppmv

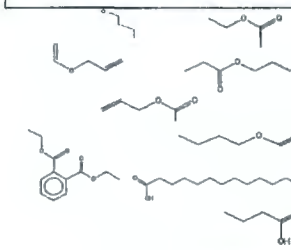
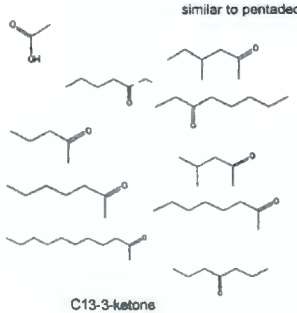
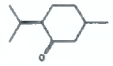
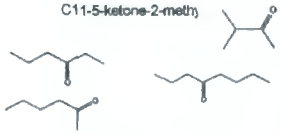
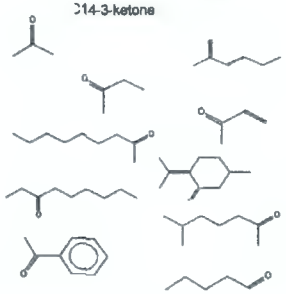
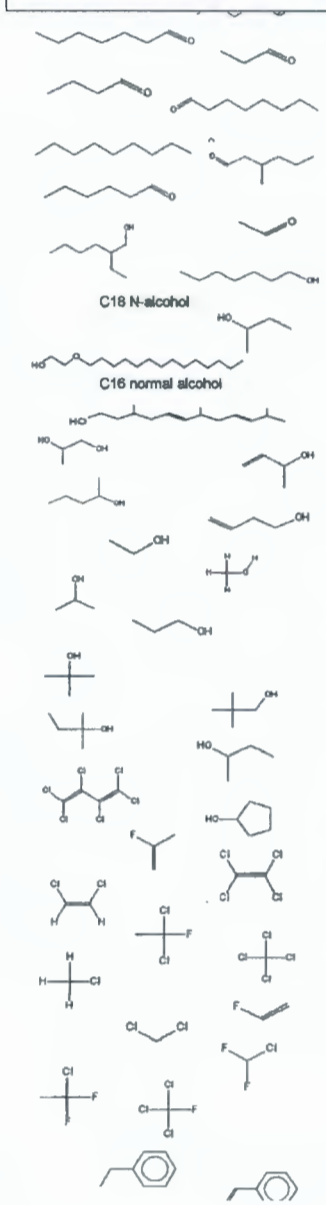
Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
	43	Acetic acid ethyl ester	88.1	141-78-6	C4H8O2	-83	77.1	8	1	482	17		
	44	Formic acid, 2-propenyl ester	86.1	1838-59-1	C4H6O2		83		6	500	25		
	45	Propanoic acid, butyl ester	130.2	590-01-2	C7H14O2	-75	145		1	427	1		
	46	Acetic acid, 2-propenyl ester	100.1	591-87-7	C5H8O2		103	"slightly"	1	475	26		
	47	Formic acid, butyl ester	102.1	592-84-7	C5H10O2	-90	107	"slightly"	1	322	1		
	48	1,2-Benzenedicarboxylic acid, diethyl ester	222.2	84-66-2	C12H14O4	-3	298	0.0896	1	540	22		
	49	Pentadecanoic acid	242.4	1002-84-2	C15H30O2	52	339		1	400	27		
	50	Butanoic acid	88.1	107-92-6	C4H8O2	-7.9	163.5	soluble	1	450	1		
	51	9-Hexadecenoic acid	254.4	2091-29-4	C16H30O2		350		7	400	27		boiling pt estimated by hexadecanoic acid
similar to pentadecanoic acid	52	Tetradecanoic acid	228.4	544-63-8	C14H28O2	53.9	326		8	400	27		
similar to pentadecanoic acid	53	Hexadecanoic acid	256.4	57-10-3	C16H32O2	62	399		5	400	27		
	54	Acetic acid	60.1	64-19-7	C2H4O2	16.3	118	miscible	5	465	1		
	55	2-Hexanone, 4-methyl-	114.2	105-42-0	C7H14O		140		5	457	28		
	56	3-Heptanone	114.2	106-35-4	C7H14O		147		5	390	17		
	57	3-Octanone	128.2	106-68-3	C8H16O		166		5	525	28		
	58	2-Pentanone	86.1	107-87-9	C5H10O	-77	102		5	505	1		
	59	2-Pentanone, 4-methyl- (MIBK)	100.2	108-10-1	C6H12O	-80	117.4		1	457	13		
	60	2-Heptanone	114.2	110-43-0	C7H14O	-35	150		5	533	13		
	61	2-Octanone	128.2	111-13-7	C8H16O	-21	173		5	525	28		
	62	2-Undecanone	170.3	112-12-9	C11H22O	17	229		5	400	27		
	63	4-Heptanone	114.2	123-19-3	C7H14O	-33	144		5	533	28		
C13-3-ketone	64	3-Tridecanone	198.4	1534-26-5	C13H26O	31	263		5*	400	27		boiling pt estimated by 2-tridecanone
C12-3-ketone	65	3-Dodecanone	184.3	1534-27-6	C12H24O	20	250		5*	400	27		boiling pt estimated by 2-tridecanone
	66	Cyclohexanone, 5-methyl-2-(1-methylethylide	152.2	15932-80-6	C10H16O	<25	224		8	500	29		
C13-6-ketone	67	6-Tridecanone	198.4	22026-12-6	C13H26O		263		6*	400	27		boiling pt estimated from 2-tridecanone (phys prop ref 6)
C11-3-ketone	68	3-Undecanone	170.3	2216-87-7	C11H22O	12	227		5	400	27		
C11-5-ketone-2-meth	69	5-Undecanone, 2-methyl-	184.3	50639-02-6	C12H24O		210		7	400	27		
	70	2-Butanone, 3-methyl-	86.1	563-80-4	C5H10O	-93	94		5	500	30		
	71	3-Hexanone	100.2	589-38-8	C6H12O	-55.6	123		5	533	28		
	72	4-Octanone	128.2	589-63-9	C8H16O		166		5	525	28		
	73	2-Hexanone	100.2	591-78-6	C6H12O	-57	127		5	533	23		
C13-2-ketone	74	2-Tridecanone	198.4	593-08-8	C13H26O		255		5	400	27		
C14-3-ketone	75	3-Tetradecanone	212.4	629-23-2	C14H28O		263		5*	400	27		boiling pt estimated by 2-tridecanone
	76	2-Propanone	58.1	67-64-1	C3H6O	-95	56		5	465	1		
	77	3-Hexen-2-one	98.1	763-93-9	C6H10O		140		8	550	28		
	78	2-Butanone	72.1	78-93-3	C4H8O	-86	80	25.6	1	516	1		
	79	3-Buten-2-one	70.1	78-94-4	C4H6O		82		5	550	31		
	80	2-Nonanone	142.2	821-55-6	C9H18O	-67	195		5	500	32		
	81	Cyclohexanone, 5-methyl-2-(1-methylethylide	152.2	89-82-7	C10H16O	<25	224		8	500	29		
	82	3-Nonanone	142.2	925-78-0	C9H18O	-8	188		1	500	32		
	83	2-Heptanone, 6-methyl-	128.2	928-68-7	C8H16O		165		5	525	28		
	84	Ethanone, 1-phenyl-	120.2	98-86-2	C8H8O	19.6	201.7	0.55	1	571	1		
	85	Pentanal	86.1	110-62-3	C5H10O	-91.5	103	0.1	1	222	23		

Table 1-2 Compounds detected > 0.1 ppmv



Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
	86	Heptanal	114.2	111-71-7	C7H14O	-43	153	<0.1	1	300	33		
	87	Propanal	58.1	123-38-6	C3H6O	-81	49	10	1	207	1		
	88	Butanal	72.1	123-72-8	C4H8O	-96	76	<0.1	1	230	1		
	89	Octanal	128.2	124-13-0	C8H16O	12	171		1	300	33		
	90	Nonanal	142.2	124-19-6	C9H18O	63	191	<0.1	8	300	33		
	91	Hexanal, 3-methyl-	114.2	19269-28-4	C7H14O		143		8	200	33		
	92	Hexanal	100.2	66-25-1	C6H12O	-56	131		1	300	33		
	93	Acetaldehyde	44.1	75-07-0	C2H4O	-124	20.1	miscible	1	175	1		
	94	1-Hexanol, 2-ethyl-	130.2	104-76-7	C8H18O	-76	183	0.1	1	300	34		
	95	1-Heptanol	116.2	111-70-6	C7H16O	-36	176		1	320	34		
	96	1-Octadecanol	270.5	112-92-5	C18H38O	61	336		1	300	34		
	97	2-Butanol	74.1	14898-79-4	C4H10O	-114	100		1	406	1		
	98	Ethanol, 2-(tetradecyloxy)-	258.4	2136-70-1	C16H34O2		253		7	300	34		boiling pt estimated by tetradecane
	99	1-Hexadecanol	242.4	36653-82-4	C16H34O	49	344		6	300	34		
	100	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	224.4	51411-24-6	C15H28O		216		7	300	34		boiling pt estimated by dodecane
	101	1,2-Propanediol	76.1	57-55-6	C3H8O2	-59	187.6	>10	1	371	1		
	102	3-Buten-2-ol	72.1	598-32-3	C4H8O		96		1	450	36		
	103	2-Pentanol	88.2	6032-29-7	C5H12O	-50	118		1	343	1		
	104	3-Buten-1-ol	72.1	627-27-0	C4H8O		113		1	450	36		
	105	Ethanol	46.1	64-17-5	C2H6O	-114	78.3	miscible	1	423	1		
	106	Methanol	32.0	67-56-1	CH4O	-98	64.6	miscible	1	470	1		
	107	2-Propanol	60.1	67-63-0	C3H8O	-88.5	82.4	miscible	1	399	23		
	108	1-Propanol	60.1	71-23-8	C3H8O	-128	97.2	miscible	1	440	1		
	109	2-Propanol, 2-methyl-	74.1	75-65-0	C4H10O	25.5	82.2	miscible	1	480	1		
	110	1-Propanol, 2,2-dimethyl-	88.2	75-84-3	C5H12O	50	113		1	480	36		
	111	2-Butanol, 2-methyl-	88.2	75-85-4	C5H12O	-12	102		1	437	1		
	112	2-Butanol	74.1	78-92-2	C4H10O	-115	99.5	15	1	406	1		
	113	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	260.8	87-68-3	C4Cl6	-21	210	0.00032	1	610	1		
	114	Cyclopentanol	86.1	96-41-3	C5H10O	-19	139	slightly	1	350	37		
	115	1-Propene, 2-fluoro-	60.1	1184-60-7	C3H5F		-24		8	600	35		
	116	Ethene, tetrachloro-	165.8	127-18-4	C2Cl4	-22.3	121.1	0.015	1	871	40	0	flammability of zero is from MSDS - JTBaker (http://www.rose-
	117	Ethene, 1,2-dichloro-, (Z)-	96.9	156-59-2	C2H2Cl2	-80.5	60	0.08	1	460	38		
	118	Ethane, 1,1-dichloro-1-fluoro- (freon 14b)	117.0	1717-00-6	C2H3Cl2F	-104	32	0.17	6	550	42	0	flammability of zero is from MSDS- Static Specialists Co. (flammability of zero is from MSDS)
	119	Methane, tetrachloro-	153.8	56-23-5	CCl4	-22.9	76.7	0.0805	1	900	41	3	described as non-flammable by phys property source 6 - rating of 3 is for evolved gases
	120	Methane, chloro- (R-40)	50.5	74-87-3	CH3Cl	-97	-24.2	0.5325	1	662	40		
	121	Ethene, fluoro-	46.0	75-02-5	C2H3F	-161	-72	insoluble	6	385	42		
	122	Methane, dichloro-	84.9	75-09-2	CH2Cl2	-96.7	39.8	5-Jan	6	662	42		
	123	Methane, chlorodifluoro- (R-22)	86.5	75-45-6	CHClF2	-146	-40.8	0.3	6	632	42		
	124	Ethane, 1-chloro-1,1-difluoro- (R-142)	100.5	75-68-3	C2H3ClF2	-131	-10	slightly	6	632	42		
	125	Methane, trichlorofluoro- (R-11)	137.4	75-69-4	CCl3F	-111	23.7	0.1	6	900	41	0	
	126	Benzene, (1-methylpentyl)-	162.3	6031-02-3	C12H18		208		6	490	43		
	127	Benzene, ethyl-	106.2	100-41-4	C8H10	-94.9	136.2	0.0206	1	432	1		

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
	128	Benzene, ethenyl-	104.2	100-42-5	C8H8	-30.6	145.2	0.032	1	490	23		
	129	Benzene, 1,4-dimethyl-	106.2	106-42-3	C8H10	13.3	1.38E+02	insoluble	1	529	23		
	130	Benzene, 1,3-dimethyl-	106.2	108-38-3	C8H10	-47.8	139.1	insoluble	1	528	23		
	131	Benzene, methyl-	92.1	108-88-3	C7H8	-93	110.6	0.0526	1	482	42		
	132	Benzene, (2-methyl-2-propenyl)-	132.2	3290-53-7	C10H12	-48	183		6	490	43		
	133	Benzene, pentyl-	148.3	538-68-1	C11H16	-75	205		1	420	43		
	134	Benzene, 1-propenyl-	118.2	637-50-3	C9H10	-27.1	175.5		1	490	43		
	135	1,1`-Biphenyl, 2-methyl-	168.2	643-58-3	C13H12	-0.2	255		6	495	23		
	136	Benzene	78.1	71-43-2	C6H6	5.5	80.1	0.18	1	582	1		
	137	1,1`-Biphenyl	154.2	92-52-4	C12H10	70	255	insoluble	1	540	23		
	138	Benzene, 1,2-dimethyl-	106.2	95-47-6	C8H10	-25.2	144	insoluble	1	464	23		
	139	1-Propyne	40.1	74-99-7	C3H4	-103	-23	0.36	6	340	40		
	140	4-Nonyne	124.2	20184-91-2	C9H16		154		6	320	39		
	141	4-Undecene, 4-methyl-	168.3	61142-40-3	C12H26		193		7	500	44		boiling pt estimated by 3-undecene and 1-undecene
C16 1-normal alkene	142	1-Hexadecene	224.4	629-73-2	C16H32	4	274		1	500	44		
	143	1-Undecene, 4-methyl-	168.3	74630-39-0	C12H24		193		7	500	44		boiling pt estimated by 3-undecene and 1-undecene
	144	3-Undecene, 2-methyl-, (Z)-	168.3	74630-48-1	C12H24		193		7	500	44		boiling pt estimated by 3-undecene and 1-undecene
	145	5-Undecene, (Z)-	154.3	764-96-5	C11H22	-107	192.3		6	500	44		
	146	4,5-Nonadiene	124.2	821-74-9	C9H16		142.5		7	550	44		boiling pt estimated by 1,8-nonadiene
	147	Naphthalene, decahydro-2,3-dimethyl-	166.3	1008-80-6	C12H22		187		7	288	45		boiling pt estimated by Decahydronaphthalene
	148	Cyclohexane, methyl-	98.2	108-87-2	C7H14	-126	101	insoluble	1	250	1		
	149	Cyclohexane	84.2	110-82-7	C6H12	6.6	80.7	<0.1	1	245	1		
	150	Cyclopropane, octyl-	154.3	1472-09-9	C11H22		150.8		7	498	46		boiling pt estimated by nonane
	151	Naphthalene, decahydro-2,6-dimethyl-	166.3	1618-22-0	C12H22		187		7	288	45		boiling pt estimated by Decahydronaphthalene
	152	Cyclopropane, 1,1-dimethyl-	70.1	1630-94-0	C5H10	-109	21		1	498	46		
	153	Cyclohexane, butyl-	140.3	1678-93-9	C10H20	-75	181		1	246	23		
	154	Cyclopropane, propyl-	84.2	2415-72-7	C6H12		69		1	498	46		
	155	Cyclopentane	70.1	287-92-3	C5H10	-93.9	49.3	insoluble	1	380	1		
	156	Octane, 2-cyclohexyl-	196.4	2883-05-8	C14H28		181		7	246	47		boiling pt estimated by butylcyclohexane
	157	Cyclododecane	168.3	294-62-2	C12H24	61	239		1	235	48		
	158	Naphthalene, decahydro-2-methyl-	152.3	2958-76-1	C11H20		201		6	288	45		
	159	Cyclohexane, 1,1,3-trimethyl-	126.2	3073-66-3	C9H18	-65.7	136.6		5	320	49		
	160	Cyclopentane, 1,3-dimethyl-2-(1-methylethyl	140.3	32281-85-9	C10H20		92		7	350	49		boiling pt estimated by Cyclopentane, 1,2-dimethyl-, trans-
	161	Naphthalene, decahydro-1,2-dimethyl-	166.3	3604-14-6	C12H22		187		7	288	45		boiling pt estimated by Decahydronaphthalene
	162	Cyclopropane, 1-pentyl-2-propyl-	154.3	41977-33-7	C11H22		151		7	498	46		boiling pt estimated by nonane
	163	Cyclohexane, pentyl-	154.3	4292-92-6	C11H22	-57.5	203.7		6	270	51		
	164	Cyclobutane, ethyl-	84.2	4806-61-5	C6H12	-143	71		1	212	23		
	165	Naphthalene, decahydro-, trans-	138.3	493-02-7	C10H18	-30.4	187.3		6	288	45		
	166	Cyclohexane, 2-butyl-1,1,3-trimethyl-	182.4	54676-39-0	C13H26		203.7		7	320	49		boiling pt estimated by pentylcyclohexane
	167	Bicyclo[4.1.0]heptane, 2-methyl-7-pentyl-	180.3	55937-92-3	C13H24		203.7		7	320	49		boiling pt estimated by pentylcyclohexane
	168	Cyclopropane, methyl-	56.1	594-11-6	C4H8	-178	0.7		6	498	46		
	169	Cyclobutane, methyl-	70.1	598-61-8	C5H10	-162	36.3		6	250	50		
	170	Cyclohexane, (4-methylpentyl)-	168.3	61142-20-9	C12H24		203.7		7	270	51		boiling pt estimated by pentylcyclohexane

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
	171	Cyclohexane, (1-methylpropyl)-	140.3	7058-01-7	C10H20		179.3		6	270	51		
	172	Cyclohexane, 1,1,2-trimethyl-	126.2	7094-26-0	C9H18	-29	145.2		6	270	51		
	173	Cyclopentane, 1,2-dimethyl-, trans-	98.2	822-50-4	C7H14	-118	92		6	350	49		
	174	Undecane, 3-methyl-	170.3	1002-43-3	C12H26	-54.5	195		5*	500	44		boiling pt estimated by undecane
	175	Butane	58.1	106-97-8	C4H10	-139	-0.45	0.0061	1	405	1		
	176	Pentane, 2-methyl-	86.2	107-83-5	C6H14	-154	62	insoluble	1	306	42		
	177	Pentane, 2,4-dimethyl-	100.2	108-08-7	C7H16	-119	81		1	337	42		
	178	Pentane	72.2	109-66-0	C5H12	-130	36.1	0.04	1	260	23		
	179	Hexane	86.2	110-54-3	C6H14	-95	69	0.00095	1	225	1		
	180	Octane	114.2	111-65-9	C8H18	-56.8	126	slightly	1	220	1		
	181	Nonane	128.3	111-84-2	C9H20	-53	150.8	<0.1	1	206	42		
normal C-11 alkane	182	Undecane	156.3	1120-21-4	C11H24	-25.6	195.6	insoluble	1	202	42		
normal C-12 alkane	183	Dodecane	170.3	112-40-3	C12H26	-9.6	216.3	0.37	6	204	42		
normal C-10 alkane	184	Decane	142.3	124-18-5	C10H22	-29.7	174.1	insoluble	6	210	1		
	185	Decane, 3-methyl-	156.3	13151-34-3	C11H24	-76	190		1	225	52		
	186	Decane, 5-methyl-	156.3	13151-35-4	C11H24		190		7	225	52		boiling pt estimated by Decane, 3-methyl-
	187	Tridecane, 3-ethyl-	212.4	13286-73-2	C15H32		252		7	220	52		boiling pt estimated by tetradecane
	188	Tridecane, 6-methyl-	198.4	13287-21-3	C14H30		235		7	220	52		boiling pt estimated by tridecane
	189	Heptane	100.2	142-82-5	C7H16	-90.6	98.4	0.01	1	223	1		
	190	Heptane, 2,2,4-trimethyl-	142.3	14720-74-2	C10H22		148		1	275	52		
	191	Tridecane, 2-methyl-	198.4	1560-96-9	C14H30	-25	248		1	205	52		
	192	Undecane, 5-methyl-	170.3	1632-70-8	C12H26	-67.7	195		5*	220	52		boiling pt estimated by undecane
	193	Undecane, 2,6-dimethyl-	184.4	17301-23-4	C13H28		195		7	250	52		boiling pt estimated by undecane
	194	Undecane, 2,8-dimethyl-	184.4	17301-25-6	C13H28		195		7	250	52		boiling pt estimated by undecane
	195	Undecane, 2,10-dimethyl-	184.4	17301-27-8	C13H28		195		7	250	52		boiling pt estimated by undecane
	196	Undecane, 3,7-dimethyl-	184.4	17301-29-0	C13H28		195		7	250	52		boiling pt estimated by undecane
	197	Undecane, 3,8-dimethyl-	184.4	17301-30-3	C13H28		195		7	250	52		boiling pt estimated by undecane
	198	Undecane, 4,7-dimethyl-	184.4	17301-32-5	C13H28		195		7	250	52		boiling pt estimated by undecane
	199	Nonane, 4-methyl-	142.3	17301-94-9	C10H22	-99	165.7		6	220	52		
	200	Nonane, 2,6-dimethyl-	156.3	17302-28-2	C11H24		165		7	250	52		boiling pt estimated by 4-methyl nonane
	201	Nonane, 3,7-dimethyl-	156.3	17302-32-8	C11H24		165		7	250	52		boiling pt estimated by 4-methyl nonane
	202	Decane, 2,5-dimethyl-	170.3	17312-50-4	C12H26	-61.8	195		5*	250	52		boiling pt estimated by undecane
	203	Dodecane, 3-methyl-	184.4	17312-57-1	C13H28	-59.4	216		5*	220	52		boiling pt estimated by dodecane
	204	Undecane, 6-ethyl-	184.4	17312-60-6	C13H28		216		7	220	52		boiling pt estimated by dodecane
	205	Undecane, 5,5-dimethyl-	184.4	17312-73-1	C13H28		216		7	250	52		boiling pt estimated by dodecane
	206	Undecane, 6,6-dimethyl-	184.4	17312-76-4	C13H28		216		7	250	52		boiling pt estimated by dodecane
	207	Undecane, 2,3-dimethyl-	184.4	17312-77-5	C13H28		216		7	250	52		boiling pt estimated by dodecane
	208	Undecane, 2,4-dimethyl-	184.4	17312-80-0	C13H28		216		7	250	52		boiling pt estimated by dodecane
	209	Undecane, 4,6-dimethyl-	184.4	17312-82-2	C13H28		216		7	250	52		boiling pt estimated by dodecane
	210	Undecane, 5-ethyl-	184.4	17453-94-0	C13H28		216		7	220	52		boiling pt estimated by dodecane
	211	Heptane, 2,3,5-trimethyl-	142.3	20278-85-7	C10H22		160.7		6	275	52		
	212	Heptane, 2,4-dimethyl-	128.3	2213-23-2	C9H20		133		1	330	52		
	213	Octane, 3-methyl-	128.3	2216-33-3	C9H20	-108	144		1	220	23		

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			
	214	Octane, 4-methyl-	128.3	2216-34-4	C9H20	-113	142		1	220	23		
	215	Tetradecane, 4-methyl-	212.4	25117-24-2	C15H32	-33	253.7		5*	220	52		boiling pt estimated by tetradecane
	216	Tridecane, 5-methyl-	198.4	25117-31-1	C14H30	-53.5	235		5*	220	52		boiling pt estimated by tridecane
	217	Tridecane, 4-methyl-	198.4	26730-12-1	C14H30	-45.7	235		5*	220	52		boiling pt estimated by tridecane
	218	Tridecane, 7-methyl-	198.4	26730-14-3	C14H30	-37.2	235		6*	225	52		boiling pt estimated by tridecane
	219	Decane, 4-methyl-	156.3	2847-72-5	C11H24	-77.5	187		6	225	52		
	220	Undecane, 4-methyl-	170.3	2980-69-0	C12H26	-66.5	210		5	220	52		
	221	Dodecane, 2,6,11-trimethyl-	212.4	31295-56-4	C15H32		252		7	250	52		boiling pt is estimated by Dodecane, 2,6,10-trimethyl-
	222	Dodecane, 2,6,10-trimethyl-	212.4	3891-98-3	C15H32		252		5	250	52		
	223	Heptane, 2,3,6-trimethyl-	142.3	4032-93-3	C10H22		156		1	275	52		
	224	Heptane, 3-ethyl-5-methyl-	142.3	52896-90-9	C10H22		158.2		6	275	52		
normal C16 alkane	225	Hexadecane	226.4	544-76-3	C16H34	18.2	287	insoluble	6	202	23		
	226	Tridecane, 4,8-dimethyl-	212.4	55030-62-1	C15H32		253.7		7	250	52		boiling pt estimated by tetradecane
	227	Dodecane, 2-methyl-8-propyl-	226.4	55045-07-3	C16H34		253.7		7	250	52		boiling pt estimated by tetradecane
	228	Tridecane, 5-propyl-	226.4	55045-11-9	C18H38		253.7		7	225	52		boiling pt estimated by tetradecane
	229	Pentane, 3,3-dimethyl-	100.2	562-49-2	C7H16	-135	90		5	350	52		
	230	Dodecane, 2,5-dimethyl-	198.4	56292-65-0	C14H30		235		7	225	52		boiling pt estimated by tridecane
	231	Pentane, 2,3-dimethyl-	100.2	565-59-3	C7H16	-134	90		5	337	42		
	232	Hexane, 3-methyl-	100.2	589-34-4	C7H16	-119	92		1	280	23		
	233	Hexane, 2,4-dimethyl-	114.2	589-43-5	C8H18		109		1	437	42		
	234	Heptane, 4-methyl-	114.2	589-53-7	C8H18	-121	118		1	250	52		
	235	Heptane, 3-methyl-	114.2	589-81-1	C8H18	-121	119		1	239	42		
	236	Hexane, 2-methyl-	100.2	591-76-4	C7H16	-118	90		1	280	23		
	237	Heptane, 2-methyl-	114.2	592-27-8	C8H18	-109	118	insoluble	6	247	42		
	238	Dodecane, 4,6-dimethyl-	198.4	61141-72-8	C14H30		235		7	225	52		boiling pt estimated by tridecane
	239	Dodecane, 4-methyl-	184.4	6117-97-1	C13H28		216		7	220	52		boiling pt estimated by dodecane
	240	3-Ethylpentane	100.2	617-78-7	C7H16	-119	93		1	275	52		
	241	Octane, 2,3,3-trimethyl-	156.3	62016-30-2	C11H24		174		7	290	52		boiling pt estimated by decane
	242	Octane, 2,3,7-trimethyl-	156.3	62016-34-6	C11H24		174		7	290	52		boiling pt estimated by decane
	243	Decane, 6-ethyl-2-methyl-	184.4	62108-21-8	C13H28		216		7	275	52		boiling pt estimated by dodecane
	244	Decane, 2,6,7-trimethyl-	184.4	62108-25-2	C13H28		216		7	290	52		boiling pt estimated by dodecane
	245	Decane, 2,4,6-trimethyl-	184.4	62108-27-4	C13H28		216		7	290	52		boiling pt estimated by dodecane
	246	Decane, 2,3,7-trimethyl-	184.4	62238-13-5	C13H28		216		7	290	52		boiling pt estimated by dodecane
C-14 alkane	247	Tridecane	184.4	629-50-5	C13H28	-5.5	235.4		1	202	42		
C-15 alkane	248	Tetradecane	198.4	629-59-4	C14H30	5.9	253.7		1	200	23		
C-17 alkane	249	Pentadecane	212.4	629-62-9	C15H32	9.9	270.6		1	202	42		
	250	Heptadecane	240.5	629-78-7	C17H36	22	301.8		1	202	42		
	251	Propane	44.1	74-98-6	C3H8	-188	-42	0.01	1	450	1		
	252	Propane, 2-methyl-	58.1	75-28-5	C4H10	-255	-11.7	slightly	6	462	1		
	253	Butane, 2-methyl-	72.2	78-78-4	C5H12	-160	30	<0.1	1	420	42		
	254	Pentane, 3-methyl-	86.2	96-14-0	C6H14	-118	64	insoluble	6	278	23		
	255	Pentane, trimethyl-, isomer	114.3	565-75-3	C8H18	-109	113.5		1	427	42		

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			

Notes

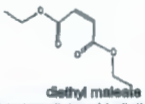
1 "quotes" imply the information is shown as written in the source
2 this compound was assigned two different CAS numbers in TWINS
* boiling point was estimated based on criteria of physical property source #7 and the available melting pt of the compound

pysical property sources

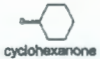
1 chemfinder (http://chemfinder.cambridgesoft.com/)
2 msds (http://www.unitexchemical.com/MSD/Uniplex214.htm)
3 estimated from msds for tetramethylcyclotetrasiloxane (http://www.schumacher.com/products/msds/tomcat_0926.pdf)
4 esimated from 2(3H)-Furanone, dihydro-5-methyl- msds (http://www.pschem.com/MSDS/pdf/GammaValerolactonePENN.PDF)
5 National Instutute of Standards and Technology (NIST) database (http://webbook.nist.gov)
6 University of Akron - Chemical Database (http://ull.chemistry.uakron.edu/erd/)
7 values estimated from similar structures - boiling pt is reported conservatively low as to not overstate adsorption potential on activated carbon
8 Interactive PhysProp Database Demo: (http://esc.syrres.com/interkow/physdemo.htm)

AIT sources (estimates are considered conservatively high based on trends within similar chemical structures)

1 Lange's Handbook of Chemistry - 14th edition
2 estimated from msds for tetramethylcyclotetrasiloxane (http://www.schumacher.com/products/msds/tomcat_0926.pdf)
3 estimated from pyridine which has same root structure - in general, alkane substitutions on any root will lower the AIT
4 estimated from 2-nitrobutane (reference 2 shows 1-nitropropane AIT is 420, nitroethane is 414, nitromethane is 418)
5 estimated from nitric acid ethyl ester (90 deg C) and nitric acid propyl ester (175 deg C)
6 estimated based on pyrolidine and tetrahydrofuran
7 estimated from MSDS which shows this compound is explosive when heated (Matheson Tri-Gas MSDS)
8 Estimated from nitrous acid -butyl ester (butyl nitrite)
9 estimated from nitric acid - propyl ester -shown with an AIT of 175 deg C by reference 2
10 estimated from tetrahydrofuran - accounting for double bonds (e.g. cyclo hexane AIT=245, benzene=562 and butane = 405, 1,3-butadiene = 420)
11 estimated from pyradine and benzene (AIT 482 and 562 respectively) accounting for the nitrogen reactivity to help oxidize the molecule
12 estimated from BASF technical data sheet (http://www.basf.com/businesses/chemicals/diols/pdfs/dihydro.pdf) showing 3,4-dihydro-2H-pyran AIT of 240 deg C.
13 estimated from 2(3H)-Furanone, dihydro-
14 estimated based on ethylene oxide AIT=429, this compound is expected to have lower AIT based on the alkane branch
15 estimated from pyridine and taking into acount that there is no resonant structure containing double bonds
16 estimated from trimethylamine AIT of 190 deg C
17 AIT reference is on COPC sheet
18 safety data from (http://physchem.ox.ac.uk/MSDS/BU/butyronitrile.html)
19 estimated based on propanenitrile and butanenitrile - in general, as the alkane chain grows, the AIT will decrease
20 estimated based on butanoic acid - alkane esters will lower the AIT below 450 deg C as shown by reference 2
21 estimated to be less than 400 deg C based on length of alkane chain
22 estimated from dimethyl phthalate and dibutylphthalate 556 and 403 deg C respectively - shown in reference 23
23 Rules of Thumb for Chemical Engineers, Gulf Publishing 1994, by Carl Branan
24 estimated from diethyl maleate (see structure on left) AIT = 350 deg C shown by reference 23
25 estimated from ethyl formate AIT of 455 deg C from reference 23
26 estimated from propyl acetate AIT of 450 deg C from reference 23
27 estimated from stearic acid (heptadecanoic (C17) acid) AIT of 395 deg C from reference 23 - this is considered valid for all of the longer chain carboxylic acids, esters, and keytones.
28 estimated from MIBK (4-methyl-2-pentanone) and 2-heptanone (AIT=457, and 533 deg C respectively) from reference 23
29 estimated from methyl phenyl ketone and cyclohexanone (AIT 570 and 420 repsectively) from reference 23 - see structures to left
30 estimated from butanone (AIT=516 deg C) considering the extra methyl substitution as an element which lowers the AIT
31 estimated from butanone (AIT=516 deg C) considering the double bond which raises the AIT
32 estimated from heptanone and nonane (AIT = 533 and 190 deg C respectively) from reference 1 - accounting for the longer alkane chain which will lower the AIT from that of heptanone
33 estimated from the trend of AITs for increasing alkane chain length within available aldehydes from reference 23
34 estimated from 1-dodecanol (AIT=275) and the trend of AIT temperature which increases as the alkane chain length decreases
35 estimated from ethyl chloride, propyl chloride, 1-2-dichloropropane, dichloroethylene, hexachlorobutadiene, and perfluorodimethylcyclohexane
36 estimated from 2-butanol, isopropyl alcohol, and 2-pentanol from reference 23
37 estimated based on cyclohexanol (AIT=300 deg C) from reference 23
38 taken from OSHA Safety and Heath Guideline database: (http://www.osha-slc.gov/SLTC/healthguidelines/1_2-dichloroethylene/recognition.html)
39 estimated from acetylene and similar length alkene from reference 1 (i.e. decene AIT = 244 deg C)
40 see AIT sources for COPCs
41 AIT for this compound can not be found - available references for safety data and MSDS indicate the compound is not flammable - to show that no credit will be taken for destruction via oxidation, the AIT is reported as 900 deg C
42 University of Akron - Chemical Database (http://ull.chemistry.uakron.edu/erd/)
43 estimated from isoproyl benzene, styrene, and butyl benzene from reference 23
44 estimated from 2-methylundecane from reference 23, however the general trend for long chain branched alkanes is a low AIT - this value (500 deg C) is considered unreasonable high - it is used here to be most conservative
45 estimated from decahydronaphthalene from reference 23 (288 deg C) -the methyl substitutions will lower the AIT
46 estimated from cyclopropane (AIT = 498 deg C)- long alkane substitution should appreciably lower the AIT
47 estimated from octylcyclohexane, cyclohexane, and methylcyclohexane from reference 1 and 23 (AIT=236, 245, and 250 respectively)



diethyl maleate
(2-batenedioic acid, diethyl ester)



cyclohexanone

methyl phenyl ketone

Table 1-2 Compounds detected > 0.1 ppmv

Structure (some obvious structures are not shown due to chain length)	no. of compounds	Chemical Name	Molecular Weight	Chemical Id	formula	melting pt	normal boiling pt	(water) solubility[1]	phys prop source	AIT	AIT source	NFPA flammability rating	Comments
		UNITS				°C	°C	g/100 ml		°C			

48 estmated from cyclo decane (AIT=235 deg C from reference 23)
49 estimated from methyl cyclopentane, hexylcyclopentane, and 1,2,4 and 1,3,5 trimethylcyclohexane from reference 23
50 estimated from ethyl cyclobutane from reference 23
51 estimated from propylcyclohexane from reference 23 (AIT = 269 deg C)
52 estimated from reference 23 which shows AIT for common alkanes, and their single, double and triple branched derivatives - not all compounds are represented, however general trends appear and all AITs (except methane) are below 500 deg C
53 estimated from reference 42 indication that this compound is a flammable solid
54 estimated from the compound structure - no data or similar compound data were found available - the 800 deg C estimate will ensure that the compound is conservatively accounted for (Benzene AIT is 562 deg C and referenceable amines range from the low 300 deg C to mid 600 deg C for aromatic amines)

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Attachment 2 Tables of Destruction DFs

Table 2-1 COPCs
Table 2-2 Compounds Detected >0.1 ppmv

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Table 2-1 COPCs

no. of compound	CAS #	COPC Compound	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
1	100-00-5	p-Nitrochlorobenzene	950.0	650.0	99.99	10000
2	100-21-0	p-Phthalic acid	1250.0	350.0	95	20
3	100-41-4	Ethyl benzene	810.0	790.0	99.99	10000
4	100-42-5	Styrene	915.0	685.0	99.99	10000
5	10061-01-5	cis-1,3-Dichloropropene	1112.0	488.0	99	100
6	10061-02-6	trans-1,3-Dichloropropene	1130.0	470.0	98	50
7	101-55-3	4-Bromophenylphenyl ether	1542.0	58.0	70	3.33
8	101-84-8	Diphenyl ether	1144.0	456.0	98	50
9	106-35-4	3-Heptanone	734.0	866.0	99.99	10000
10	106-42-3	p-Xylene (Dimethyl benzene)	986.0	614.0	99.9	1000
11	106-46-7	1,4-Dichlorobenzene	1184.0	416.0	98	50
12	106-88-7	1,2-Epoxybutane	894.2	705.8	99.99	10000
13	106-93-4	Ethylene dibromide (Dibromoethane)	1600.0	0.0	0	1
14	106-97-8	Butane (R-600)	761.0	839.0	99.99	10000
15	106-99-0	1,3-Butadiene	840.2	759.8	99.99	10000
16	107-02-8	Acrolein	455.0	1145.0	99.99	10000
17	107-05-1	3-Chloropropene (Allyl chloride)	905.0	695.0	99.99	10000
18	107-06-2	1,2-Dichloroethane (Ethylene chloride) (freon 150)	773.6	826.4	99.99	10000
19	107-12-0	Propionitrile	950.0	650.0	99.99	10000
20	107-13-1	Acrylonitrile	897.8	702.2	99.99	10000
21	107-18-6	2-Propene-1-ol	712.4	887.6	99.99	10000
22	107-31-3	Formic acid, methyl ester	869.0	731.0	99.99	10000
23	107-66-4	Dibutylphosphate	950.0	650.0	99.99	10000
24	107-87-9	2-Pentanone	941.0	659.0	99.99	10000
25	108-03-2	1-Nitropropane	788.0	812.0	99.99	10000
26	108-05-4	Vinyl acetate	800.6	799.4	99.99	10000
27	108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	858.0	742.0	99.99	10000
28	108-20-3	Bis(isopropyl)ether	829.0	771.0	99.99	10000
29	108-38-3	m-Xylene (Dimethyl benzene)	986.0	614.0	99.9	1000
30	108-39-4	m-Cresol	1038.2	561.8	99.9	1000
31	108-87-2	Methylcyclohexane	482.0	1118.0	99.99	10000
32	108-88-3	Toluene	896.0	704.0	99.99	10000
33	108-90-7	Chlorobenzene	1245.0	355.0	95	20
34	108-93-0	Cyclohexanol	572.0	1028.0	99.99	10000
35	108-94-1	Cyclohexanone	788.0	812.0	99.99	10000
36	108-95-2	Phenol	1319.0	281.0	90	10
37	109-66-0	n-Pentane	500.0	1100.0	99.99	10000
38	109-99-9	Tetrahydrofuran	609.8	990.2	99.99	10000
39	110-12-3	5-Methyl-2-hexanone	376.0	1224.0	99.99	10000
40	110-43-0	2-Heptanone	739.0	861.0	99.99	10000

Table 2-1 COPCs

no. of compound	CAS #	COPC Compound	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
41	110-54-3	n-Hexane	437.0	1163.0	99.99	10000
42	110-62-3	n-Valeraldehyde	500.0	1100.0	99.99	10000
43	110-82-7	Cyclohexane	473.0	1127.0	99.99	10000
44	110-83-8	Cyclohexene	590.0	1010.0	99.99	10000
45	110-86-1	Pyridine	899.6	700.4	99.99	10000
46	111-65-9	n-Octane	428.0	1172.0	99.99	10000
47	111-76-2	Ethylene glycol monobutyl ether	460.4	1139.6	99.99	10000
48	111-84-2	n-Nonane	374.0	1226.0	99.99	10000
49	117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	734.0	866.0	99.99	10000
50	117-84-0	n-Dioctyl phthalate	735.1	864.9	99.99	10000
51	120-12-7	Anthracene	1000.4	599.6	99.9	1000
52	120-82-1	1,2,4-Trichlorobenzene	1060.0	540.0	99	100
53	120-83-2	2,4-Dichlorophenol	1542.0	58.0	70	3.33
54	121-44-8	Triethylamine	480.0	1120.0	99.99	10000
55	121-69-7	Dimethylaniline	699.8	900.2	99.99	10000
56	122-39-4	N,N-Diphenylamine	1173.0	427.0	98	50
57	123-19-3	4-Heptanone	842.0	758.0	99.99	10000
58	123-38-6	n-Propionaldehyde	404.6	1195.4	99.99	10000
59	123-51-3	3-Methyl-1-butanol	662.0	938.0	99.99	10000
60	123-86-4	Acetic acid n-butyl ester	797.0	803.0	99.99	10000
61	123-91-1	1,4-Dioxane	356.0	1244.0	99.99	10000
62	126-73-8	Tributyl phosphate	899.6	700.4	99.99	10000
63	126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	860.0	740.0	99.99	10000
64	127-18-4	Perchloroethylene (tetrachloroethylene)	1600.0	0.0	0	1
65	127-19-5	N,N-Dimethylacetamide	914.0	686.0	99.99	10000
66	128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	878.0	722.0	99.99	10000
67	129-00-0	Pyrene	1542.0	58.0	70	3.33
68	1321-64-8	Pentachloronaphthalene	1542.0	58.0	70	3.33
69	1321-65-9	Trichloronaphthalene	1542.0	58.0	70	3.33
70	132-64-9	Dibenzofuran	1542.0	58.0	70	3.33
71	1335-87-1	Hexachloronaphthalene	1542.0	58.0	70	3.33
72	1335-88-2	Tetrachloronaphthalene	1542.0	58.0	70	3.33
73	1336-36-3	Polychlorinated biphenyls (PCBs)	1542.0	58.0	70	3.33
74	141-78-6	Acetic acid ethyl ester (Ethyl acetate)	906.8	693.2	99.99	10000
75	141-79-7	4-Methyl-3-penten-2-one	651.0	949.0	99.99	10000
76	142-82-5	n-Heptane	433.4	1166.6	99.99	10000
77	144-62-7	Oxalic acid	1400.0	200.0	90	10
78	156-60-5	trans-1,2-Dichloroethylene	860.0	740.0	99.99	10000
79	1634-04-4	Methyl tert-butyl ether	815.0	785.0	99.99	10000
80	189-55-9	Dibenzo[a,i]pyrene	1542.0	58.0	70	3.33

Table 2-1 COPCs

no. of compound	CAS #	COPC Compound	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
81	189-64-0	Dibenzo[a,h]pyrene	1542.0	58.0	70	3.33
82	191-24-2	Benzo(g,h,i)perylene	1542.0	58.0	70	3.33
83	191-30-0	Benzo[a,i]pyrene	1542.0	58.0	70	3.33
84	192-65-4	Dibenzo[a,e]pyrene	1542.0	58.0	70	3.33
85	193-39-5	Indeno(1,2,3-cd)pyrene	1542.0	58.0	70	3.33
86	206-44-0	Fluoranthene	1542.0	58.0	70	3.33
87	208-96-8	Acenaphthylene	1542.0	58.0	70	3.33
88	2234-13-1	Octachloronaphthalene	1542.0	58.0	70	3.33
89	224-42-0	Dibenz[a,j]acridine	1542.0	58.0	70	3.33
90	226-36-8	Dibenz[a,h]acridine	1542.0	58.0	70	3.33
91	25551-13-7	Trimethyl benzene	1022.0	578.0	99.9	1000
92	26140-60-3	Terphenyls	1542.0	58.0	70	3.33
93	27154-33-2	Trichlorofluoroethane	1600.0	0.0	0	1
94	287-92-3	Cyclopentane	716.0	884.0	99.99	10000
95	3697-24-3	5-Methylchrysene	1542.0	58.0	70	3.33
96	3825-26-1	Ammonium perfluorooctanoate	1542.0	58.0	70	3.33
97	4170-30-3	2-Butenaldehyde (2-Butenal)	446.0	1154.0	99.99	10000
98	50-00-0	Formaldehyde	806.0	794.0	99.99	10000
99	50-32-8	Benzo(a)pyrene	1542.0	58.0	70	3.33
100	53-70-3	Dibenzo(a,h)anthracene	1542.0	58.0	70	3.33
101	540-59-0	1,2-Dichloroethylene	860.0	740.0	99.99	10000
102	540-84-1	2,2,4-Trimethylpentane	779.0	821.0	99.99	10000
103	541-73-1	1,3-Dichlorobenzene	1184.0	416.0	98	50
104	56-23-5	Carbon tetrachloride (R-10)	1600.0	0.0	0	1
105	563-80-4	3-Methyl-2-butanone	845.6	754.4	99.99	10000
106	56-49-5	3-Methylcholanthrene	1542.0	58.0	70	3.33
107	57-14-7	1,1-Dimethylhydrazine	480.2	1119.8	99.99	10000
108	58-90-2	2,3,4,6-Tetrachlorophenol	1542.0	58.0	70	3.33
109	591-78-6	2-Hexanone	991.0	609.0	99.9	1000
110	59-50-7	4-Chloro-3-methylphenol	1542.0	58.0	70	3.33
111	59-89-2	N-Nitrosomorpholine	932.0	668.0	99.99	10000
112	602-87-9	5-Nitroacenaphthene	1542.0	58.0	70	3.33
113	60-29-7	Ethyl ether	320.0	1280.0	99.99	10000
114	603-34-9	Triphenylamine	1542.0	58.0	70	3.33
115	60-34-4	Methylhydrazine	384.8	1215.2	99.99	10000
116	60-35-5	Acetamide	896.0	704.0	99.99	10000
117	621-64-7	Di-n-Propylnitrosamine	527.0	1073.0	99.99	10000
118	624-83-9	Methyl isocyanate	995.0	605.0	99.9	1000
119	627-13-4	Nitric acid, propyl ester	788.0	812.0	99.99	10000
120	62-75-9	N-Nitroso-N,N-dimethylamine	932.0	668.0	99.99	10000

Table 2-1 COPCs

no. of compound	CAS #	COPC Compound	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
121	630-20-6	1,1,1,2-Tetrachloroethane	1600.0	0.0	0	1
122	64-17-5	Ethyl alcohol	798.8	801.2	99.99	10000
123	64-18-6	Formic acid	813.2	786.8	99.99	10000
124	64-19-7	Acetic acid	869.0	731.0	99.99	10000
125	67-56-1	Methyl alcohol (Methanol)	878.0	722.0	99.99	10000
126	67-63-0	2-Propyl alcohol (Isopropanol)	852.8	747.2	99.99	10000
127	67-64-1	2-Propanone (Acetone)	869.0	731.0	99.99	10000
128	67-66-3	Chloroform (R-20)	1832.0	-232.0	0	1
129	67-72-1	Hexachloroethane	1600.0	0.0	0	1
130	684-16-2	Hexafluoroacetone	1600.0	0.0	0	1
131	71-23-8	n-Propyl alcohol	824.0	776.0	99.99	10000
132	71-36-3	n-Butyl alcohol	692.6	907.4	99.99	10000
133	71-43-2	Benzene	1097.6	502.4	99	100
134	71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	999.0	601.0	99.9	1000
135	74-83-9	Bromomethane (Methyl bromide) (halon 1001)	998.6	601.4	99.9	1000
136	74-87-3	Chloromethane (Methyl chloride) (R-40)	1223.6	376.4	95	20
137	74-97-5	Bromochloromethane (halon 1011)	1600.0	0.0	0	1
138	74-99-7	Methylacetylene	644.0	956.0	99.99	10000
139	75-00-3	Chloroethane	966.2	633.8	99.9	1000
140	75-01-4	Vinyl chloride (1-Chloroethene)	881.6	718.4	99.99	10000
141	75-05-8	Acetonitrile	975.2	624.8	99.9	1000
142	75-07-0	Acetaldehyde	347.0	1253.0	99.99	10000
143	75-09-2	Dichloromethane (Methylene chloride) (R-30)	1223.6	376.4	95	20
144	75-12-7	Formamide	932.0	668.0	99.99	10000
145	75-15-0	Carbon disulfide	257.0	1343.0	99.99	10000
146	75-21-8	Ethylene oxide (Oxirane)	804.2	795.8	99.99	10000
147	75-27-4	Bromodichloromethane	1600.0	0.0	0	1
148	75-34-3	1,1-Dichloroethane	852.8	747.2	99.99	10000
149	75-35-4	1,1-Dichloroethene (Vinylidene chloride)	854.6	745.4	99.99	10000
150	75-43-4	Dichlorofluoromethane (R-21)	1026.0	574.0	99.9	1000
151	75-45-6	Chlorodifluoromethane (R-22)	1170.0	430.0	98	50
152	75-50-3	Trimethylamine	374.0	1226.0	99.99	10000
153	75-52-5	Nitromethane	784.4	815.6	99.99	10000
154	75-55-8	2-Methylaziridine	914.0	686.0	99.99	10000
155	75-61-6	Difluorodibromomethane (freon 12B2- halon 1202)	1600.0	0.0	0	1
156	75-63-8	Trifluorobromomethane (R-13B1)	1600.0	0.0	0	1
157	75-65-0	2-Methyl-2-propanol	892.4	707.6	99.99	10000
158	75-69-4	Trichlorofluoromethane (R-11)	1600.0	0.0	0	1
159	75-71-8	Dichlorodifluoromethane (R-12)	1600.0	0.0	0	1
160	76-03-9	Trichloroacetic acid	1600.0	0.0	0	1

Table 2-1 COPCs

no. of compound	CAS #	COPC Compound	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
161	76-11-9	1,1,1,2-Tetrachloro-2,2-difluoroethane (R-112a)	1350.0	250.0	90	10
162	76-12-0	1,1,2,2-Tetrachloro-1,2-difluoroethane (R-112)	1350.0	250.0	90	10
163	76-13-1	1,2,2-Trichloro-1,1,2-trifluoroethane (Freon 113)	1256.0	344.0	95	20
164	76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane (R-114)	1600.0	0.0	0	1
165	76-15-3	Chloropentafluoroethane (R-115)	1600.0	0.0	0	1
166	78-83-1	2-Methylpropyl alcohol (Isobutyl alcohol)	779.0	821.0	99.99	10000
167	78-87-5	1,2-Dichloropropane	1034.0	566.0	99.9	1000
168	78-92-2	1-Methylpropyl alcohol (2-Butanol)	762.8	837.2	99.99	10000
169	78-93-3	Methyl ethyl ketone (MEK, 2-Butanone)	960.8	639.2	99.9	1000
170	79-00-5	1,1,2-Trichloroethane	932.0	668.0	99.99	10000
171	79-01-6	Trichloroethylene	788.0	812.0	99.99	10000
172	79-09-4	Propionic acid	914.0	686.0	99.99	10000
173	79-10-7	2-Propenoic acid	820.4	779.6	99.99	10000
174	79-20-9	Methyl acetate	935.6	664.4	99.99	10000
175	79-34-5	1,1,2,2-Tetrachloroethane	1600.0	0.0	0	1
176	83-32-9	Acenaphthene	1542.0	58.0	70	3.33
177	84-66-2	Diethyl phthalate	855.0	745.0	99.99	10000
178	84-74-2	Dibutyl phthalate	756.0	844.0	99.99	10000
179	85-01-8	Phenanthrene	1542.0	58.0	70	3.33
180	85-68-7	Butylbenzyl phthalate	451.4	1148.6	99.99	10000
181	86-73-7	Fluorene	1542.0	58.0	70	3.33
182	87-68-3	Hexachlorobutadiene	1130.0	470.0	98	50
183	88-06-2	2,4,6-Trichlorophenol	1542.0	58.0	70	3.33
184	88-72-2	2-Nitrotoluene	581.0	1019.0	99.99	10000
185	88-75-5	2-Nitrophenol	1542.0	58.0	70	3.33
186	88-89-1	Picric acid	572.0	1028.0	99.99	10000
187	91-20-3	Naphthalene	1054.0	546.0	99	100
188	91-22-5	Quinoline	896.0	704.0	99.99	10000
189	91-58-7	2-Chloronapthalene	1542.0	58.0	70	3.33
190	92-52-4	1,1`-Biphenyl	1004.0	596.0	99.9	1000
191	92-93-3	4-Nitrobiphenyl	1542.0	58.0	70	3.33
192	95-13-6	Indene	979.0	621.0	99.9	1000
193	95-47-6	o-Xylene	869.0	731.0	99.99	10000
194	95-48-7	o-Cresol (2-Methylphenol)	1038.2	561.8	99.9	1000
195	95-49-8	2-Chlorotoluene	932.0	668.0	99.99	10000
196	95-50-1	o-Dichlorobenzene (1,2-Dichlorobenzene)	1184.0	416.0	98	50
197	95-57-8	2-Chlorophenol	779.0	821.0	99.99	10000
198	95-95-4	2,4,5-Trichlorophenol	1542.0	58.0	70	3.33
199	96-18-4	1,2,3-Trichloropropane	932.0	668.0	99.99	10000
200	96-22-0	3-Pentanone	842.0	758.0	99.99	10000

Table 2-1 COPCs

no. of compound	CAS #	COPC	AIT	RTO degrees above AIT	est DE	est DF
		Compound	deg F	deg F	%	mass in / mass out
201	96-69-5	Bis(3-tert-butyl-4-hydroxy-6-methyl-phenyl)sulfide	1542.0	58.0	70	3.33
202	98-51-1	p-tert-Butyltoluene	950.0	650.0	99.99	10000
203	98-82-8	Cumene	795.0	805.0	99.99	10000
204	98-83-9	alpha-Methylstyrene	1065.2	534.8	99	100
205	98-86-2	Acetophenone	1059.8	540.2	99	100
206	98-95-3	Nitrobenzene	899.6	700.4	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

		headspace detects >0.1 ppmv	AIT	AIT	RTO degrees above AIT	est DE	est DF
no of compound	CAS #	Compound name	deg C	deg F	deg F	%	mass in / mass out
1	541-05-9	Cyclotrisiloxane, hexamethyl-	400	752	848	99.99	10000
2	556-67-2	Cyclotetrasiloxane, octamethyl-	400	752	848	99.99	10000
3	USI000-06	tetramethylcyclotrisiloxane	250	482	1118	99.99	10000
4	3622-84-2	Benzenesulfonamide, N-butyl-	800	1472	128	80	5
5	5145-07-1	2(3H)-Furanone, dihydro-3,5-dimethyl-	425	797	803	99.99	10000
6	108-47-4	Pyridine, 2,4-dimethyl-	482	899.6	700.4	99.99	10000
7	109-99-9	Furan, tetrahydro-	321	609.8	990.2	99.99	10000
8	110-00-9	Furan	360	680	920	99.99	10000
9	110-86-1	Pyridine	482	899.6	700.4	99.99	10000
10	1708-29-8	Furan, 2,5-dihydro-	450	842	758	99.99	10000
11	24405-16-1	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	350	662	938	99.99	10000
12	289-95-2	Pyrimidine	450	842	758	99.99	10000
13	290-37-9	Pyrazine	450	842	758	99.99	10000
14	534-22-5	Furan, 2-methyl-	450	842	758	99.99	10000
15	930-22-3	Oxirane, ethenyl-	429	804.2	795.8	99.99	10000
16	96-48-0	2(3H)-Furanone, dihydro- (gamma butyrolactone)	450	842	758	99.99	10000
17	3457-90-7	1,3-Propanediol, dinitrate	450	842	758	99.99	10000
18	3457-91-8	1,4-Butanediol, dinitrate	450	842	758	99.99	10000
19	544-16-1	Nitrous acid, butyl ester	450	842	758	99.99	10000
20	624-91-9	Nitrous acid, methyl ester	500	932	668	99.99	10000
21	625-58-1	Nitric acid, ethyl ester	90	194	1406	99.99	10000
22	627-05-4	Butane, 1-nitro-	450	842	758	99.99	10000
23	627-13-4	Nitric acid, propyl ester	175	347	1253	99.99	10000
24	62-75-9M	Methanamine, N-methyl-N-nitroso- and others	500	932	668	99.99	10000
25	928-45-0	Nitric acid, butyl ester	400	752	848	99.99	10000
26	123-75-1	Pyrrolidine	450	842	758	99.99	10000
27	22431-09-0	Methanamine, N-(1-methylbutylidene)-	350	662	938	99.99	10000
28	616-45-5	2-Pyrrolidinone	450	842	758	99.99	10000
29	75-50-3	Methanamine, N,N-dimethyl-	190	374	1226	99.99	10000
30	107-12-0	Propanenitrile	510	950	650	99.99	10000
31	109-74-0	Butanenitrile	488	910.4	689.6	99.99	10000
32	110-59-8	Pentanenitrile	475	887	713	99.99	10000
33	124-12-9	Octanenitrile	450	842	758	99.99	10000
34	2243-27-8	Nonanenitrile	440	824	776	99.99	10000
35	628-73-9	Hexanenitrile	470	878	722	99.99	10000
36	629-08-3	Heptanenitrile	460	860	740	99.99	10000
37	75-05-8	Acetonitrile	524	975.2	624.8	99.9	1000
38	109-21-7	Butanoic acid, butyl ester	450	842	758	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	headspace detects >0.1 ppmv Compound name	AIT deg C	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
39	110-27-0	Tetradecanoic acid, 1-methylethyl ester	400	752	848	99.99	10000
40	123-25-1	Butanedioic acid, diethyl ester	350	662	938	99.99	10000
41	123-86-4	Acetic acid, butyl ester	425	797	803	99.99	10000
42	126-73-8	Phosphoric acid tributyl ester	482	899.6	700.4	99.99	10000
43	141-78-6	Acetic acid ethyl ester	482	899.6	700.4	99.99	10000
44	1838-59-1	Formic acid, 2-propenyl ester	500	932	668	99.99	10000
45	590-01-2	Propanoic acid, butyl ester	427	800.6	799.4	99.99	10000
46	591-87-7	Acetic acid, 2-propenyl ester	475	887	713	99.99	10000
47	592-84-7	Formic acid, butyl ester	322	611.6	988.4	99.99	10000
48	84-66-2	1,2-Benzenedicarboxylic acid, diethyl ester	540	1004	596	99.9	1000
49	1002-84-2	Pentadecanoic acid	400	752	848	99.99	10000
50	107-92-6	Butanoic acid	450	842	758	99.99	10000
51	2091-29-4	9-Hexadecenoic acid	400	752	848	99.99	10000
52	544-63-8	Tetradecanoic acid	400	752	848	99.99	10000
53	57-10-3	Hexadecanoic acid	400	752	848	99.99	10000
54	64-19-7	Acetic acid	465	869	731	99.99	10000
55	105-42-0	2-Hexanone, 4-methyl-	457	854.6	745.4	99.99	10000
56	106-35-4	3-Heptanone	390	734	866	99.99	10000
57	106-68-3	3-Octanone	525	977	623	99.9	1000
58	107-87-9	2-Pentanone	505	941	659	99.99	10000
59	108-10-1	2-Pentanone, 4-methyl- (MIBK)	457	854.6	745.4	99.99	10000
60	110-43-0	2-Heptanone	533	991.4	608.6	99.9	1000
61	111-13-7	2-Octanone	525	977	623	99.9	1000
62	112-12-9	2-Undecanone	400	752	848	99.99	10000
63	123-19-3	4-Heptanone	533	991.4	608.6	99.9	1000
64	1534-26-5	3-Tridecanone	400	752	848	99.99	10000
65	1534-27-6	3-Dodecanone	400	752	848	99.99	10000
66	15932-80-6	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-	500	932	668	99.99	10000
67	22026-12-6	6-Tridecanone	400	752	848	99.99	10000
68	2216-87-7	3-Undecanone	400	752	848	99.99	10000
69	50639-02-6	5-Undecanone, 2-methyl-	400	752	848	99.99	10000
70	563-80-4	2-Butanone, 3-methyl-	500	932	668	99.99	10000
71	589-38-8	3-Hexanone	533	991.4	608.6	99.9	1000
72	589-63-9	4-Octanone	525	977	623	99.9	1000
73	591-78-6	2-Hexanone	533	991.4	608.6	99.9	1000
74	593-08-8	2-Tridecanone	400	752	848	99.99	10000
75	629-23-2	3-Tetradecanone	400	752	848	99.99	10000
76	67-64-1	2-Propanone	465	869	731	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	headspace detects >0.1 ppmv Compound name	AIT deg C	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
77	763-93-9	3-Hexen-2-one	550	1022	578	99.9	1000
78	78-93-3	2-Butanone	516	960.8	639.2	99.9	1000
79	78-94-4	3-Buten-2-one	550	1022	578	99.9	1000
80	821-55-6	2-Nonanone	500	932	668	99.99	10000
81	89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)	500	932	668	99.99	10000
82	925-78-0	3-Nonanone	500	932	668	99.99	10000
83	928-68-7	2-Heptanone, 6-methyl-	525	977	623	99.9	1000
84	98-86-2	Ethanone, 1-phenyl-	571	1059.8	540.2	99	100
85	110-62-3	Pentanal	222	431.6	1168.4	99.99	10000
86	111-71-7	Heptanal	300	572	1028	99.99	10000
87	123-38-6	Propanal	207	404.6	1195.4	99.99	10000
88	123-72-8	Butanal	230	446	1154	99.99	10000
89	124-13-0	Octanal	300	572	1028	99.99	10000
90	124-19-6	Nonanal	300	572	1028	99.99	10000
91	19269-28-4	Hexanal, 3-methyl-	200	392	1208	99.99	10000
92	66-25-1	Hexanal	300	572	1028	99.99	10000
93	75-07-0	Acetaldehyde	175	347	1253	99.99	10000
94	104-76-7	1-Hexanol, 2-ethyl-	300	572	1028	99.99	10000
95	111-70-6	1-Heptanol	320	608	992	99.99	10000
96	112-92-5	1-Octadecanol	300	572	1028	99.99	10000
97	14898-79-4	2-Butanol	406	762.8	837.2	99.99	10000
98	2136-70-1	Ethanol, 2-(tetradecyloxy)-	300	572	1028	99.99	10000
99	36653-82-4	1-Hexadecanol	300	572	1028	99.99	10000
100	51411-24-6	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	300	572	1028	99.99	10000
101	57-55-6	1,2-Propanediol	371	699.8	900.2	99.99	10000
102	598-32-3	3-Buten-2-ol	450	842	758	99.99	10000
103	6032-29-7	2-Pentanol	343	649.4	950.6	99.99	10000
104	627-27-0	3-Buten-1-ol	450	842	758	99.99	10000
105	64-17-5	Ethanol	423	793.4	806.6	99.99	10000
106	67-56-1	Methanol	470	878	722	99.99	10000
107	67-63-0	2-Propanol	399	750.2	849.8	99.99	10000
108	71-23-8	1-Propanol	440	824	776	99.99	10000
109	75-65-0	2-Propanol, 2-methyl-	480	896	704	99.99	10000
110	75-84-3	1-Propanol, 2,2-dimethyl-	480	896	704	99.99	10000
111	75-85-4	2-Butanol, 2-methyl-	437	818.6	781.4	99.99	10000
112	78-92-2	2-Butanol	406	762.8	837.2	99.99	10000
113	87-68-3	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	610	1130	470	98	50
114	96-41-3	Cyclopentanol	350	662	938	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	headspace detects >0.1 ppmv Compound name	AIT deg C	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
115	1184-60-7	1-Propene, 2-fluoro-	600	1112	488	99	100
116	127-18-4	Ethene, tetrachloro-	871	1599.8	0.2	0	1
117	156-59-2	Ethene, 1,2-dichloro-, (Z)-	460	860	740	99.99	10000
118	1717-00-6	Ethane, 1,1-dichloro-1-fluoro- (freon 14b)	550	1022	578	99.9	1000
119	56-23-5	Methane, tetrachloro-	900	1652	-52	0	1
120	74-87-3	Methane, chloro- (R-40)	662	1223.6	376.4	95	20
121	75-02-5	Ethene, fluoro-	385	725	875	99.99	10000
122	75-09-2	Methane, dichloro-	662	1223.6	376.4	95	20
123	75-45-6	Methane, chlorodifluoro- (R-22)	632	1169.6	430.4	98	50
124	75-68-3	Ethane, 1-chloro-1,1-difluoro- (R-142)	632	1169.6	430.4	98	50
125	75-69-4	Methane, trichlorofluoro- (R-11)	900	1652	-52	0	1
126	6031-02-3	Benzene, (1-methylpentyl)-	490	914	686	99.99	10000
127	100-41-4	Benzene, ethyl-	432	809.6	790.4	99.99	10000
128	100-42-5	Benzene, ethenyl-	490	914	686	99.99	10000
129	106-42-3	Benzene, 1,4-dimethyl-	529	984.2	615.8	99.9	1000
130	108-38-3	Benzene, 1,3-dimethyl-	528	982.4	617.6	99.9	1000
131	108-88-3	Benzene, methyl-	482	899.6	700.4	99.99	10000
132	3290-53-7	Benzene, (2-methyl-2-propenyl)-	490	914	686	99.99	10000
133	538-68-1	Benzene, pentyl-	420	788	812	99.99	10000
134	637-50-3	Benzene, 1-propenyl-	490	914	686	99.99	10000
135	643-58-3	1,1`-Biphenyl, 2-methyl-	495	923	677	99.99	10000
136	71-43-2	Benzene	562	1043.6	556.4	99.9	1000
137	92-52-4	1,1`-Biphenyl	540	1004	596	99.9	1000
138	95-47-6	Benzene, 1,2-dimethyl-	464	867.2	732.8	99.99	10000
139	74-99-7	1-Propyne	340	644	956	99.99	10000
140	20184-91-2	4-Nonyne	320	608	992	99.99	10000
141	61142-40-3	4-Undecene, 4-methyl-	500	932	668	99.99	10000
142	629-73-2	1-Hexadecene	500	932	668	99.99	10000
143	74630-39-0	1-Undecene, 4-methyl-	500	932	668	99.99	10000
144	74630-48-1	3-Undecene, 2-methyl-, (Z)-	500	932	668	99.99	10000
145	764-96-5	5-Undecene, (Z)-	500	932	668	99.99	10000
146	821-74-9	4,5-Nonadiene	550	1022	578	99.9	1000
147	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	288	550.4	1049.6	99.99	10000
148	108-87-2	Cyclohexane, methyl-	250	482	1118	99.99	10000
149	110-82-7	Cyclohexane	245	473	1127	99.99	10000
150	1472-09-9	Cyclopropane, octyl-	498	928.4	671.6	99.99	10000
151	1618-22-0	Naphthalene, decahydro-2,6-dimethyl-	288	550.4	1049.6	99.99	10000
152	1630-94-0	Cyclopropane, 1,1-dimethyl-	498	928.4	671.6	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

		headspace detects >0.1 ppmv	AIT	AIT	RTO degrees above AIT	est DE	est DF
no of compound	CAS #	Compound name	deg C	deg F	deg F	%	mass in / mass out
153	1678-93-9	Cyclohexane, butyl-	246	474.8	1125.2	99.99	10000
154	2415-72-7	Cyclopropane, propyl-	498	928.4	671.6	99.99	10000
155	287-92-3	Cyclopentane	380	716	884	99.99	10000
156	2883-05-8	Octane, 2-cyclohexyl-	246	474.8	1125.2	99.99	10000
157	294-62-2	Cyclododecane	235	455	1145	99.99	10000
158	2958-76-1	Naphthalene, decahydro-2-methyl-	288	550.4	1049.6	99.99	10000
159	3073-66-3	Cyclohexane, 1,1,3-trimethyl-	320	608	992	99.99	10000
160	32281-85-9	Cyclopentane, 1,3-dimethyl-2-(1-methylethyl)-	350	662	938	99.99	10000
161	3604-14-6	Naphthalene, decahydro-1,2-dimethyl-	288	550.4	1049.6	99.99	10000
162	41977-33-7	Cyclopropane, 1-pentyl-2-propyl-	498	928.4	671.6	99.99	10000
163	4292-92-6	Cyclohexane, pentyl-	270	518	1082	99.99	10000
164	4806-61-5	Cyclobutane, ethyl-	212	413.6	1186.4	99.99	10000
165	493-02-7	Naphthalene, decahydro-, trans-	288	550.4	1049.6	99.99	10000
166	54676-39-0	Cyclohexane, 2-butyl-1,1,3-trimethyl-	320	608	992	99.99	10000
167	55937-92-3	Bicyclo[4.1.0]heptane, 2-methyl-7-pentyl-	320	608	992	99.99	10000
168	594-11-6	Cyclopropane, methyl-	498	928.4	671.6	99.99	10000
169	598-61-8	Cyclobutane, methyl-	250	482	1118	99.99	10000
170	61142-20-9	Cyclohexane, (4-methylpentyl)-	270	518	1082	99.99	10000
171	7058-01-7	Cyclohexane, (1-methylpropyl)-	270	518	1082	99.99	10000
172	7094-26-0	Cyclohexane, 1,1,2-trimethyl-	270	518	1082	99.99	10000
173	822-50-4	Cyclopentane, 1,2-dimethyl-, trans-	350	662	938	99.99	10000
174	1002-43-3	Undecane, 3-methyl-	500	932	668	99.99	10000
175	106-97-8	Butane	405	761	839	99.99	10000
176	107-83-5	Pentane, 2-methyl-	306	582.8	1017.2	99.99	10000
177	108-08-7	Pentane, 2,4-dimethyl-	337	638.6	961.4	99.99	10000
178	109-66-0	Pentane	260	500	1100	99.99	10000
179	110-54-3	Hexane	225	437	1163	99.99	10000
180	111-65-9	Octane	220	428	1172	99.99	10000
181	111-84-2	Nonane	206	402.8	1197.2	99.99	10000
182	1120-21-4	Undecane	202	395.6	1204.4	99.99	10000
183	112-40-3	Dodecane	204	399.2	1200.8	99.99	10000
184	124-18-5	Decane	210	410	1190	99.99	10000
185	13151-34-3	Decane, 3-methyl-	225	437	1163	99.99	10000
186	13151-35-4	Decane, 5-methyl-	225	437	1163	99.99	10000
187	13286-73-2	Tridecane, 3-ethyl-	220	428	1172	99.99	10000
188	13287-21-3	Tridecane, 6-methyl-	220	428	1172	99.99	10000
189	142-82-5	Heptane	223	433.4	1166.6	99.99	10000
190	14720-74-2	Heptane, 2,2,4-trimethyl-	275	527	1073	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	headspace detects >0.1 ppmv Compound name	AIT deg C	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
191	1560-96-9	Tridecane, 2-methyl-	205	401	1199	99.99	10000
192	1632-70-8	Undecane, 5-methyl-	220	428	1172	99.99	10000
193	17301-23-4	Undecane, 2,6-dimethyl-	250	482	1118	99.99	10000
194	17301-25-6	Undecane, 2,8-dimethyl-	250	482	1118	99.99	10000
195	17301-27-8	Undecane, 2,10-dimethyl-	250	482	1118	99.99	10000
196	17301-29-0	Undecane, 3,7-dimethyl-	250	482	1118	99.99	10000
197	17301-30-3	Undecane, 3,8-dimethyl-	250	482	1118	99.99	10000
198	17301-32-5	Undecane, 4,7-dimethyl-	250	482	1118	99.99	10000
199	17301-94-9	Nonane, 4-methyl-	220	428	1172	99.99	10000
200	17302-28-2	Nonane, 2,6-dimethyl-	250	482	1118	99.99	10000
201	17302-32-8	Nonane, 3,7-dimethyl-	250	482	1118	99.99	10000
202	17312-50-4	Decane, 2,5-dimethyl-	250	482	1118	99.99	10000
203	17312-57-1	Dodecane, 3-methyl-	220	428	1172	99.99	10000
204	17312-60-6	Undecane, 6-ethyl-	220	428	1172	99.99	10000
205	17312-73-1	Undecane, 5,5-dimethyl-	250	482	1118	99.99	10000
206	17312-76-4	Undecane, 6,6-dimethyl-	250	482	1118	99.99	10000
207	17312-77-5	Undecane, 2,3-dimethyl-	250	482	1118	99.99	10000
208	17312-80-0	Undecane, 2,4-dimethyl-	250	482	1118	99.99	10000
209	17312-82-2	Undecane, 4,6-dimethyl-	250	482	1118	99.99	10000
210	17453-94-0	Undecane, 5-ethyl-	220	428	1172	99.99	10000
211	20278-85-7	Heptane, 2,3,5-trimethyl-	275	527	1073	99.99	10000
212	2213-23-2	Heptane, 2,4-dimethyl-	330	626	974	99.99	10000
213	2216-33-3	Octane, 3-methyl-	220	428	1172	99.99	10000
214	2216-34-4	Octane, 4-methyl-	220	428	1172	99.99	10000
215	25117-24-2	Tetradecane, 4-methyl-	220	428	1172	99.99	10000
216	25117-31-1	Tridecane, 5-methyl-	220	428	1172	99.99	10000
217	26730-12-1	Tridecane, 4-methyl-	220	428	1172	99.99	10000
218	26730-14-3	Tridecane, 7-methyl-	225	437	1163	99.99	10000
219	2847-72-5	Decane, 4-methyl-	225	437	1163	99.99	10000
220	2980-69-0	Undecane, 4-methyl-	220	428	1172	99.99	10000
221	31295-56-4	Dodecane, 2,6,11-trimethyl-	250	482	1118	99.99	10000
222	3891-98-3	Dodecane, 2,6,10-trimethyl-	250	482	1118	99.99	10000
223	4032-93-3	Heptane, 2,3,6-trimethyl-	275	527	1073	99.99	10000
224	52896-90-9	Heptane, 3-ethyl-5-methyl-	275	527	1073	99.99	10000
225	544-76-3	Hexadecane	202	395.6	1204.4	99.99	10000
226	55030-62-1	Tridecane, 4,8-dimethyl-	250	482	1118	99.99	10000
227	55045-07-3	Dodecane, 2-methyl-8-propyl-	250	482	1118	99.99	10000
228	55045-11-9	Tridecane, 5-propyl-	225	437	1163	99.99	10000

Table 2-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	headspace detects >0.1 ppmv Compound name	AIT deg C	AIT deg F	RTO degrees above AIT deg F	est DE %	est DF mass in / mass out
229	562-49-2	Pentane, 3,3-dimethyl-	350	662	938	99.99	10000
230	56292-65-0	Dodecane, 2,5-dimethyl-	225	437	1163	99.99	10000
231	565-59-3	Pentane, 2,3-dimethyl-	337	638.6	961.4	99.99	10000
232	589-34-4	Hexane, 3-methyl-	280	536	1064	99.99	10000
233	589-43-5	Hexane, 2,4-dimethyl-	437	818.6	781.4	99.99	10000
234	589-53-7	Heptane, 4-methyl-	250	482	1118	99.99	10000
235	589-81-1	Heptane, 3-methyl-	239	462.2	1137.8	99.99	10000
236	591-76-4	Hexane, 2-methyl-	280	536	1064	99.99	10000
237	592-27-8	Heptane, 2-methyl-	247	476.6	1123.4	99.99	10000
238	61141-72-8	Dodecane, 4,6-dimethyl-	225	437	1163	99.99	10000
239	6117-97-1	Dodecane, 4-methyl-	220	428	1172	99.99	10000
240	617-78-7	3-Ethylpentane	275	527	1073	99.99	10000
241	62016-30-2	Octane, 2,3,3-trimethyl-	290	554	1046	99.99	10000
242	62016-34-6	Octane, 2,3,7-trimethyl-	290	554	1046	99.99	10000
243	62108-21-8	Decane, 6-ethyl-2-methyl-	275	527	1073	99.99	10000
244	62108-25-2	Decane, 2,6,7-trimethyl-	290	554	1046	99.99	10000
245	62108-27-4	Decane, 2,4,6-trimethyl-	290	554	1046	99.99	10000
246	62238-13-5	Decane, 2,3,7-trimethyl-	290	554	1046	99.99	10000
247	629-50-5	Tridecane	202	395.6	1204.4	99.99	10000
248	629-59-4	Tetradecane	200	392	1208	99.99	10000
249	629-62-9	Pentadecane	202	395.6	1204.4	99.99	10000
250	629-78-7	Heptadecane	202	395.6	1204.4	99.99	10000
251	74-98-6	Propane	450	842	758	99.99	10000
252	75-28-5	Propane, 2-methyl-	462	863.6	736.4	99.99	10000
253	78-78-4	Butane, 2-methyl-	420	788	812	99.99	10000
254	96-14-0	Pentane, 3-methyl-	278	532.4	1067.6	99.99	10000
255	565-75-3	Pentane, trimethyl-, isomer	427	800.6	799.4	99.99	10000

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Attachment 3 Tables of Removal DFs

Table 3-1 COPCs
Table 3-2 Compounds Detected >0.1 ppmv

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Table 3-1 COPCs

no of compo und	CAS	Compound Name (COPC)	MW	Boiling pt.	Yaws capacity correlation carbon loading quadratic constants			assumed outlet equilibrium of isotherm-PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.10			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
			g/mol	deg C	A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
1	100-00-5	p-Nitrochlorobenzene	157.6	242							40	98	50	40	98	50
2	100-21-0	p-Phthalic acid	166.1	sublimes							40	98	50	40	98	50
4	100-41-4	Ethyl benzene	106.2	136.2							2	80	5	2	80	5
5	100-42-5	Styrene	104.1	145.2							2	80	5	2	80	5
6	10061-01-5	cis-1,3-Dichloropropene	111.0	104.3							2	80	5	2	80	5
7	10061-02-6	trans-1,3-Dichloropropene	111.0	112							2	80	5	2	80	5
8	101-55-3	4-Bromophenylphenyl ether	249.1	310.14							40	98	50	40	98	50
9	101-84-8	Diphenyl ether	170.2	498							40	98	50	40	98	50
10	106-35-4	3-Heptanone	114.2	147							2	80	5	2	80	5
11	106-42-3	p-Xylene (Dimethyl benzene)	106.2	138.3							2	80	5	2	80	5
12	106-46-7	1,4-Dichlorobenzene	147.0	173.4							10	95	20	10	95	20
13	106-88-7	1,2-Epoxybutane	72.1	63.3	0.36719	0.37654	-0.0236	0.93	(0.07)	(7.88)	1	50	2	0.5	20	1.25
14	106-93-4	Ethylene dibromide (Dibromoethane)	187.9	131.7	1.44231	0.255	-0.02666	14.48	9.48	65.46	5	90	10	5	90	10
15	106-97-8	Butane	58.1	-0.45	0.03071	0.34304	-0.01596	0.47	0.47	100.00	0	0	1	0	0	1
16	106-99-0	1,3-Butadiene	54.1	-4.4	-0.03359	0.34764	-0.01297	0.40	0.40	100.00	0	0	1	0	0	1
17	107-02-8	Acrolein	56.1	52.7	-0.29632	0.49437	-0.02471	0.15	(0.85)	(553.73)	1	50	2	0	0	1
18	107-05-1	3-Chloropropene (Allyl chloride)	76.5	44	0.32792	0.36553	-0.01853	0.88	0.38	43.10	0.5	20	1.25	0.5	20	1.25
19	107-06-2	1,2-Dichloroethane (Ethylene chloride)	99.0	83.5	0.55343	0.37072	-0.02161	1.45	0.45	30.99	1	50	2	1	50	2
20	107-12-0	Propionitrile	55.1	97.2	0.05925	0.51747	-0.03781	0.32	(0.68)	(213.35)	1	50	2	0	0	1
21	107-13-1	Acrylonitrile	53.1	77.3	0.07669	0.49986	-0.035	0.35	(0.65)	(187.19)	1	50	2	0	0	1
22	107-18-6	2-Propene-1-ol	58.1	97	0.3239	0.49368	-0.0437	0.61	(0.39)	(63.49)	1	50	2	0.5	20	1.25
23	107-31-3	Formic acid, methyl ester	60.1	32	-0.99586	0.61693	-0.01847	0.02	(0.48)	(2039.09)	0.5	20	1.25	0	0	1
24	107-66-4	Dibutylphosphate	210.2	100							2	80	5	2	80	5
25	107-87-9	2-Pentanone	86.1	100							1	50	2	1	50	2
26	108-03-2	1-Nitropropane	89.1	131	0.91328	0.34648	-0.0373	3.38	1.38	40.91	2	80	5	2	80	5
27	108-05-4	Vinyl acetate	86.1	72.3	0.61067	0.34797	-0.02595	1.72	0.72	42.02	1	50	2	1	50	2
28	108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	100.2	117.4							2	80	5	2	80	5
29	108-20-3	Bis(isopropyl)ether	102.2	66.5							1	50	2	1	50	2
30	108-38-3	m-Xylene (Dimethyl benzene)	106.2	139.1							2	80	5	2	80	5
31	108-39-4	m-Cresol	108.1	202							10	95	20	10	95	20
32	108-87-2	Methylcyclohexane	98.2	101							2	80	5	2	80	5
33	108-88-3	Toluene	92.1	110.6							2	80	5	2	80	5
34	108-90-7	Chlorobenzene	112.6	130							2	80	5	2	80	5
35	108-93-0	Cyclohexanol	100.2	161							10	95	20	10	95	20
36	108-94-1	Cyclohexanone	98.2	155.6							10	95	20	10	95	20
37	108-95-2	Phenol	94.1	181.7							10	95	20	10	95	20
38	109-66-0	n-Pentane	72.2	36.1							0.5	20	1.25	0.5	20	1.25
39	109-99-9	Tetrahydrofuran	72.1	86	0.29856	0.35648	-0.0155	0.84	(0.16)	(18.42)	1	50	2	0.5	20	1.25
40	110-12-3	5-Methyl-2-hexanone	114.2	144							2	80	5	2	80	5
41	110-43-0	2-Heptanone	114.2	150							2	80	5	2	80	5
42	110-54-3	n-Hexane	86.2	69							1	50	2	1	50	2
43	110-62-3	n-Valeraldehyde	86.1	103							2	80	5	2	80	5
44	110-82-7	Cyclohexane	84.2	80.7							1	50	2	1	50	2
45	110-83-8	Cyclohexene	82.1	83							1	50	2	1	50	2
46	110-86-1	Pyridine	79.1	115.2							2	80	5	2	80	5
47	111-85-9	n-Octane	114.2	126							2	80	5	2	80	5
48	111-76-2	Ethylene glycol monobutyl ether	118.0	171							10	95	20	10	95	20
49	111-84-2	n-Nonane	128.3	150.8							10	95	20	10	95	20
50	117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	390.5	386.9							40	98	50	40	98	50
51	117-84-0	n-Dioctyl phthalate	390.6	220							40	98	50	40	98	50
53	120-12-7	Anthracene	178.2	340							40	98	50	40	98	50

Table 3-1 COPCs

no of compo und	CAS	Compound Name (COPC)	MW	Boiling pt.	Yaws capacity correlation carbon loading quadratic constants			assumed outlet equilibrium of isotherm-PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.10			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
			g/mol	deg C	A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
54	120-82-1	1,2,4-Trichlorobenzene	181.5	214.4							40	98	50	40	98	50
55	120-83-2	2,4-Dichlorophenol	163.0	210							40	98	50	40	98	50
56	121-44-8	Triethylamine	101.2	88.9							1	50	2	1	50	2
57	121-69-7	Dimethylaniline	121.2	194							10	95	20	10	95	20
58	122-39-4	N,N-Diphenylamine	169.2	302							40	98	50	40	98	50
59	123-19-3	4-Heptanone	114.2	144							2	80	5	2	80	5
60	123-38-6	n-Propionaldehyde	58.1	49	0.05519	0.49738	-0.04331	0.33	(0.17)	(52.92)	0.5	20	1.25	0	0	1
61	123-51-3	3-Methyl-1-butanol	88.2	130							2	80	5	2	80	5
62	123-86-4	Acetic acid n-butyl ester	116.2	126.1							2	80	5	2	80	5
63	123-91-1	1,4-Dioxane	88.1	101.1	0.66781	0.36208	-0.03034	1.89	(0.11)	(6.08)	2	80	5	1	50	2
64	126-73-8	Tributyl phosphate	266.3	289							40	98	50	40	98	50
65	126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	67.1	90.3	0.46655	0.3889	-0.03042	1.11	0.11	10.30	1	50	2	1	50	2
66	127-18-4	Perchloroethylene (tetrachloroethylene)	165.9	121.1	1.40596	0.20802	-0.02097	15.03	10.03	66.73	5	90	10	5	90	10
67	127-19-5	N,N-Dimethylacetamide	87.1	166	1.20026	0.25124	-0.03263	8.25	(1.75)	(21.23)	10	95	20	5	90	10
68	128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	220.4	265							40	98	50	40	98	50
69	129-00-0	Pyrene	202.2	404							40	98	50	40	98	50
70	1321-64-8	Pentachloronaphthalene	300.4	327							40	98	50	40	98	50
71	1321-65-9	Trichloronaphthalene	231.5	304							40	98	50	40	98	50
72	132-64-9	Dibenzofuran	168.2	285							40	98	50	40	98	50
73	1335-87-1	Hexachloronaphthalene	334.8	343							40	98	50	40	98	50
74	1335-88-2	Tetrachloronaphthalene	266.0	316							40	98	50	40	98	50
75	1336-36-3	Polychlorinated biphenyls (PCBs)	322.0	>195							40	98	50	40	98	50
76	141-78-6	Acetic acid ethyl ester (Ethyl acetate)	88.1	77.1	0.63612	0.34441	-0.02691	1.84	0.84	45.65	1	50	2	1	50	2
77	141-79-7	4-Methyl-3-penten-2-one	98.2	127							2	80	5	2	80	5
78	142-82-5	n-Heptane	100.2	98.4							1	50	2	1	50	2
79	144-62-7	Oxalic acid	90.0	190							10	95	20	10	95	20
80	156-60-5	trans-1,2-Dichloroethylene	97.0	47.5	0.47567	0.39061	-0.02554	1.15	0.65	56.40	0.5	20	1.25	0.5	20	1.25
82	1634-04-4	Methyl tert-butyl ether	88.2	55.2							1	50	2	1	50	2
84	189-55-9	Dibenzo[a,i]pyrene	302.4	404							40	98	50	40	98	50
85	189-64-0	Dibenzo[a,h]pyrene	302.4	404							40	98	50	40	98	50
86	191-24-2	Benzo(g,h,i)perylene	276.3	500							40	98	50	40	98	50
87	191-30-0	Benzo[a,j]pyrene	302.4	404							40	98	50	40	98	50
88	192-65-4	Dibenzo[a,e]pyrene	302.4	sublimes							40	98	50	40	98	50
89	193-39-5	Indeno(1,2,3-cd)pyrene	276.3	536							40	98	50	40	98	50
92	206-44-0	Fluoranthene	202.3	375							40	98	50	40	98	50
94	208-96-8	Acenaphthylene	152.2	265							40	98	50	40	98	50
96	2234-13-1	Octachloronaphthalene	403.7	440							40	98	50	40	98	50
97	224-42-0	Dibenz[a,j]acridine	279.3	>346							40	98	50	40	98	50
98	226-36-8	Dibenz[a,h]acridine	279.3	>346							40	98	50	40	98	50
100	25551-13-7	Trimethyl benzene	120.2	164.7							10	95	20	10	95	20
101	26140-60-3	Terphenyls	230.3	337							40	98	50	40	98	50
102	27154-33-2	Trichlorofluoroethane	151.4	146.5							5	90	10	5	90	10
103	287-92-3	Cyclopentane	70.1	49							0.5	20	1.25	0.5	20	1.25
108	3697-24-3	5-Methylchrysene	242.3	404							40	98	50	40	98	50
109	3825-26-1	Ammonium perfluorooctanoate	431.1	192							20	98	50	20	98	50
110	4170-30-3	2-Butenaldehyde (2-Butenal)	70.1	102	0.68353	0.3656	-0.034	1.92	(0.08)	(4.02)	2	80	5	1	50	2
112	50-00-0	Formaldehyde	30.0	-19.5	-2.48524	0.69123	-0.00375	0.00	0.00	100.00	0	0	1	0	0	1
114	50-32-8	Benzo(a)pyrene	252.3	495							40	98	50	40	98	50
115	53-70-3	Dibenzo(a,h)anthracene	278.3	524							40	98	50	40	98	50
116	540-59-0	1,2-Dichloroethylene	96.9	48	0.47567	0.39061	-0.02554	1.15	0.65	56.40	0.5	20	1.25	0.5	20	1.25
117	540-84-1	2,2,4-Trimethylpentane	114.2	99.2							1	50	2	1	50	2

Table 3-1 COPCs

no of compo und	CAS	Compound Name (COPC)	MW g/mol	Boiling pt. deg C	Yaws capacity correlation carbon loading quadratic constants A	B	C	assumed outlet equilibrium of isotherm-PPMV (y) 0.10 g ads/100 g carbon	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001) Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out	estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995) Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out
118	541-73-1	1,3-Dichlorobenzene	147.0	173							10	95	20	10	95	20
119	56-23-5	Carbon tetrachloride	153.8	76.7	1.07481	0.28186	-0.02276	5.89	3.89	66.05	2	80	5	2	80	5
120	563-80-4	3-Methyl-2-butanone	86.1	94							1	50	2	1	50	2
121	56-49-5	3-Methylcholanthrene	268.4	280							40	98	50	40	98	50
123	57-14-7	1,1-Dimethylhydrazine	60.1	63							1	50	2	1	50	2
125	58-90-2	2,3,4,6-Tetrachlorophenol	231.9	150							5	90	10	5	90	10
126	591-78-6	2-Hexanone	100.2	127							2	80	5	2	80	5
127	59-50-7	4-Chloro-3-methylphenol	142.6	235							10	95	20	10	95	20
128	59-89-2	N-Nitrosomorpholine	116.1	224							10	95	20	10	95	20
129	602-87-9	5-Nitroacenaphthene	199.2	279							40	98	50	40	98	50
130	60-29-7	Ethyl ether	74.1	34.6	0.23477	0.36044	-0.02236	0.71	0.21	29.69	0.5	20	1.25	0.5	20	1.25
131	603-34-9	Triphenylamine	245.3	347							40	98	50	40	98	50
132	60-34-4	Methylhydrazine	46.1	87.8							0	0	1	0	0	1
133	60-35-5	Acetamide	59.1	221	1.23333	0.21723		10.38	0.38	3.64	10	95	20	10	95	20
135	621-64-7	Di-n-Propylnitrosamine	130.2	206							10	95	20	10	95	20
136	624-83-9	Methyl isocyanate	57.1	39	-1.07579	0.85881	-0.06876	0.01	(0.49)	(4938.83)	0.5	20	1.25	0	0	1
137	627-13-4	Nitric acid, propyl ester	105.1	110							2	80	5	2	80	5
138	62-75-9	N-Nitroso-N,N-dimethylamine	74.1	153							2	95	20	2	95	20
139	630-20-6	1,1,1,2-Tetrachloroethane	167.9	130.5							5	90	10	5	90	10
140	64-17-5	Ethyl alcohol	46.1	78.3	-0.51153	0.67525	-0.04473	0.06	0.06	100.00	0	0	1	0	0	1
141	64-18-6	Formic acid	46.0	100.7	-1.77731	1.09503	-0.06354	1.16E-03	0.00	100.00	0	0	1	0	0	1
142	64-19-7	Acetic acid	60.1	118	-0.05553	0.6841	-0.06071	0.16	(1.84)	(1162.90)	2	80	5	0	0	1
143	67-56-1	Methyl alcohol (Methanol)	32.0	64.6							0	0	1	0	0	1
144	67-63-0	2-Propyl alcohol (Isopropanol)	60.1	82.4	0.27183	0.46419	-0.03682	0.59	(0.41)	(69.50)	1	50	2	0.5	20	1.25
145	67-64-1	2-Propanone (Acetone)	58.1	56.2	-0.14546	0.47497	-0.02286	0.23	(0.77)	(339.84)	1	50	2	0	0	1
146	67-66-3	Chloroform	119.4	61.7	0.67102	0.36148	-0.02288	1.93	0.93	48.32	1	50	2	1	50	2
147	67-72-1	Hexachloroethane	236.7	sublimes							40	98	50	40	98	50
148	684-16-2	Hexafluoroacetone	166.0	-26							0	0	1	0	0	1
149	71-23-8	n-Propyl alcohol	60.1	97.2	0.38644	0.48033	-0.04505	0.73	(0.27)	(37.70)	1	50	2	0.5	20	1.25
150	71-36-3	n-Butyl alcohol	74.1	117.6	0.89881	0.32534	-0.03648	3.44	1.44	41.92	2	80	5	2	80	5
151	71-43-2	Benzene	78.1	80.1							1	50	2	1	50	2
152	71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	133.4	74.1	0.97331	0.28737	-0.02277	4.60	3.60	78.28	1	50	2	1	50	2
157	74-83-9	Bromomethane (Methyl bromide)	95.0	3.56	-1.23835	0.78564	-0.05521	0.01	0.01	100.00	0	0	1	0	0	1
158	74-87-3	Chloromethane (Methyl chloride)	50.5	-24.2	-1.91871	0.62053	-0.00549	0.00	0.00	100.00	0	0	1	0	0	1
159	74-97-5	Bromochloromethane	129.4	67.8	0.61399	0.41353	-0.02531	1.50	0.50	33.19	1	50	2	1	50	2
160	74-99-7	Methylacetylene	40.1	-23	-2.52865	1.74715	-0.21635	0.00	0.00	100.00	0	0	1	0	0	1
161	75-00-3	Chloroethane	64.5	12.3	-0.50828	0.50364	-0.02179	0.09	0.09	100.00	0	0	1	0	0	1
162	75-01-4	Vinyl chloride (1-Chloroethene)	62.5	-13.9	-0.98889	0.66564	-0.0432	0.02	0.02	100.00	0	0	1	0	0	1
163	75-05-8	Acetonitrile	41.1	81.6	-0.79666	0.63512	-0.02598	0.03	0.03	100.00	0	0	1	0	0	1
164	75-07-0	Acetaldehyde	44.1	20.1	-1.17047	0.62766	-0.02475	0.02	0.02	100.00	0	0	1	0	0	1
165	75-09-2	Dichloromethane (Methylene chloride)	84.9	39.8	-0.07043	0.4921	-0.02276	0.26	(0.24)	(92.42)	0.5	20	1.25	0	0	1
166	75-12-7	Formamide	45.0	210	1.30981	0.25274		11.40	11.40	100.00	0	0	1	0	0	1
167	75-15-0	Carbon disulfide	76.1	46.2							0.5	20	1.25	0.5	20	1.25
168	75-21-8	Ethylene oxide (Oxirane)	44.1	10.7	-2.42379	0.94878	-0.04062	0.00	0.00	100.00	0	0	1	0	0	1
169	75-27-4	Bromodichloromethane	163.8	90.1							2	80	5	2	80	5
170	75-34-3	1,1-Dichloroethane	99.0	57.3	0.54485	0.36091	-0.02192	1.45	0.45	31.14	1	50	2	1	50	2
171	75-35-4	1,1-Dichloroethene (Vinylidene chloride)	97.0	31.7							0.5	20	1.25	0.5	20	1.25
172	75-43-4	Dichlorofluoromethane	102.9	9							0	0	1	0	0	1
173	75-45-6	Chlorodifluoromethane	86.5	-40.8							0	0	1	0	0	1
174	75-50-3	Trimethylamine	59.1	2.87	-0.09422	0.32583	-0.00337	0.38	0.38	100.00	0	0	1	0	0	1
175	75-52-5	Nitromethane	61.0	101	-0.32847	0.70602	-0.05111	0.08	(1.92)	(2335.73)	2	80	5	0	0	1

Table 3-1 COPCs

no of compo und	CAS	Compound Name (COPC)	MW	Boiling pt.	Yaws capacity correlation carbon loading quadratic constants			assumed outlet equilibrium of isotherm-PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.10			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
			g/mol	deg C	A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
176	75-55-8	2-Methylaziridine	57.1	66	0.06919	0.43529	-0.02293	0.41	(0.59)	(144.92)	1	50	2	0	0	1
177	75-61-6	Difluorodibromomethane	209.8	24	0.82076	0.30701	-0.01384	3.16	3.16	100.00	0	0	1	0	0	1
178	75-63-8	Trifluorobromomethane	148.9	-57.8							0	0	1	0	0	1
179	75-65-0	2-Methyl-2-propanol	74.1	82.2							1	50	2	1	50	2
180	75-69-4	Trichlorofluoromethane	137.4	23.8	0.17307	0.40715	-0.01915	0.56	0.56	100.00	0	0	1	0	0	1
181	75-71-8	Dichlorodifluoromethane	120.9	-29.79	-0.0735	0.40145	-0.01404	0.32	0.32	100.00	0	0	1	0	0	1
183	76-03-9	Trichloroacetic acid	163.4	196							20	98	50	20	98	50
184	76-11-9	1,1,1,2-Tetrachloro-2,2-difluoroethane	203.8	91							2	80	5	2	80	5
185	76-12-0	1,1,2,2-Tetrachloro-1,2-difluoroethane	203.8	93	1.37307	0.17625	-0.01465	15.21	13.21	86.85	2	80	5	2	80	5
186	76-13-1	1,2,2-Trichloro-1,1,2-trifluoroethane (Freon 113)	187.4	47.6	1.27368	0.18656	-0.01231	11.88	10.88	91.58	1	50	2	1	50	2
187	76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane	170.9	3.8							0	0	1	0	0	1
188	76-15-3	Chloropentafluoroethane	154.5	-39.1	0.08264	0.34756	-0.01343	0.53	0.53	100.00	0	0	1	0	0	1
190	78-83-1	2-Methylpropyl alcohol (Isobutyl alcohol)	74.1	107.9	0.84818	0.33155	-0.03559	3.03	1.03	33.93	2	80	5	2	80	5
191	78-87-5	1,2-Dichloropropane	113.0	96.8	0.98872	0.287	-0.02571	4.74	3.74	78.91	1	50	2	1	50	2
192	78-92-2	1-Methylpropyl alcohol (2-Butanol)	74.1	99.5	0.76814	0.34611	-0.03478	2.44	1.44	59.00	1	50	2	1	50	2
193	78-93-3	Methyl ethyl ketone (MEK, 2-Butanone)	72.1	79.6	0.46525	0.37688	-0.02801	1.15	0.15	12.98	1	50	2	1	50	2
194	79-00-5	1,1,2-Trichloroethane	133.4	113.8	1.17163	0.27791	-0.02746	7.35	5.35	72.79	2	80	5	2	80	5
195	79-01-6	Trichloroethylene	131.4	86.7	1.02411	0.29929	-0.02539	5.01	4.01	80.02	1	50	2	1	50	2
196	79-09-4	Propionic acid	74.1	140.7	0.77846	0.4457	-0.05209	1.91	(0.09)	(4.80)	2	80	5	1	50	2
197	79-10-7	2-Propenoic acid	72.1	141.6	0.75549	0.47108	-0.05615	1.69	(0.31)	(18.24)	2	80	5	1	50	2
198	79-20-9	Methyl acetate	74.1	56.9	0.13314	0.42849	-0.02188	0.48	(0.52)	(107.60)	1	50	2	0	0	1
199	79-34-5	1,1,2,2-Tetrachloroethane	167.9	146.3	1.52322	0.17848	-0.02019	21.11	16.11	76.32	5	90	10	5	90	10
202	83-32-9	Acenaphthene	154.2	279							40	98	50	40	98	50
203	84-66-2	Diethyl phthalate	222.2	298							40	98	50	40	98	50
204	84-74-2	Dibutyl phthalate	278.3	340							40	98	50	40	98	50
205	85-01-8	Phenanthrene	178.2	340							40	98	50	40	98	50
206	85-68-7	Butylbenzyl phthalate	312.4	370							40	98	50	40	98	50
207	86-73-7	Fluorene	166.2	295							40	98	50	40	98	50
208	87-68-3	Hexachlorobutadiene	260.8	210							40	98	50	40	98	50
210	88-06-2	2,4,6-Trichlorophenol	197.5	244.5							40	98	50	40	98	50
211	88-72-2	2-Nitrotoluene	137.1	221							10	95	20	10	95	20
212	88-75-5	2-Nitrophenol	139.1	214.6							10	95	20	10	95	20
214	88-89-1	Picric acid	229.1	>300							40	98	50	40	98	50
215	91-20-3	Naphthalene	128.2	218							10	95	20	10	95	20
216	91-22-5	Quinoline	129.2	238							10	95	20	10	95	20
217	91-58-7	2-Chloronapthalene	162.6	256							40	98	50	40	98	50
218	92-52-4	1,1`-Biphenyl	154.2	255							40	98	50	40	98	50
219	92-93-3	4-Nitrobiphenyl	199.2	340							40	98	50	40	98	50
223	95-13-6	Indene	116.2	181.6							10	95	20	10	95	20
224	95-47-6	o-Xylene	106.2	144							2	80	5	2	80	5
225	95-48-7	o-Cresol (2-Methylphenol)	108.1	191							10	95	20	10	95	20
226	95-49-8	2-Chlorotoluene	126.6	159							10	95	20	10	95	20
227	95-50-1	o-Dichlorobenzene (1,2-Dichlorobenzene)	147.0	180.5							10	95	20	10	95	20
228	95-57-8	2-Chlorophenol	128.6	175.6							10	95	20	10	95	20
229	95-95-4	2,4,5-Trichlorophenol	197.5	253							40	98	50	40	98	50
230	96-18-4	1,2,3-Trichloropropane	147.4	156	1.47241	0.18136	-0.02165	18.60	8.60	46.22	10	95	20	10	95	20
231	96-22-0	3-Pentanone	86.1	101							2	80	5	2	80	5
232	96-69-5	Bis(3-tert-butyl-4-hydroxy-6-methyl-phenyl)sulfide	358.5	316							40	98	50	40	98	50
233	98-51-1	p-tert-Butyltoluene	148.3	193							10	95	20	10	95	20
234	98-82-8	Cumene	120.2	151							10	95	20	10	95	20
235	98-83-9	alpha-Methylstyrene	118.2	165.4							10	95	20	10	95	20

Table 3-1 COPCs

no of compo und	CAS	Compound Name (COPC)	MW	Boiling pt.	Yaws capacity correlation carbon loading quadratic constants			assumed outlet equilibrium of isotherm-PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.10			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
			g/mol	deg C	A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
236	98-86-2	Acetophenone	120.5	201.7							10	95	20	10	95	20
237	98-95-3	Nitrobenzene	123.1	210.8							10	95	20	10	95	20

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.100			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
					A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
1	541-05-9	Cyclotrisiloxane, hexamethyl-	222.5	134							5	90	10	5	90	10
2	556-67-2	Cyclotetrasiloxane, octamethyl-	296.6	175							20	98	50	20	98	50
3	USI000-06	tetramethylcyclotrisiloxane	194.0	135							5	90	10	5	90	10
4	3622-84-2	Benzenesulfonamide, N-butyl-	213.3	314							40	98	50	40	98	50
5	5145-07-1	2(3H)-Furanone, dihydro-3,5-dimethyl-	114.1	206							10	95	20	10	95	20
6	108-47-4	Pyridine, 2,4-dimethyl-	107.2	159							10	95	20	10	95	20
7	109-99-9	Furan, tetrahydro-	72.1	66	0.29856	0.35648	-0.0155	0.844	(0.156)	-18.42	1	50	2	0.5	20	1.25
8	110-00-9	Furan	68.1	31.4	0.04084	0.40613	-0.0162	0.415	(0.085)	-20.35	0.5	20	1.25	0	0	1
9	110-86-1	Pyridine	79.1	115.2							2	80	5	2	80	5
10	1708-29-8	Furan, 2,5-dihydro-	70.1	67	0.3399	0.40041	-0.02451	0.822	(0.178)	-21.62	1	50	2	0.5	20	1.25
11	24405-16-	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	128.2	180							10	95	20	10	95	20
12	289-95-2	Pyrimidine	80.1	123							2	80	5	2	80	5
13	290-37-9	Pyrazine	80.1	115							2	80	5	2	80	5
14	534-22-5	Furan, 2-methyl-	82.1	63							1	50	2	1	50	2
15	930-22-3	Oxirane, ethenyl-	70.1	67							1	50	2	1	50	2
16	96-48-0	2(3H)-Furanone, dihydro- (gamma butyrolactone)	86.1	205	1.29434	0.29719	-0.04658	8.924	(1.076)	-12.05	10	95	20	5	90	10
17	3457-90-7	1,3-Propanediol, dinitrate	166.1	100							2	80	5	2	80	5
18	3457-91-8	1,4-Butanediol, dinitrate	180.1	130							5	90	10	5	90	10
19	544-16-1	Nitrous acid, butyl ester	103.1	78							1	50	2	1	50	2
20	624-91-9	Nitrous acid, methyl ester	61.0	64.6							1	50	2	1	50	2
21	625-58-1	Nitric acid, ethyl ester	91.1	88							1	50	2	1	50	2
22	627-05-4	Butane, 1-nitro-	103.1	153							10	95	20	10	95	20
23	627-13-4	Nitric acid, propyl ester	105.1	110							2	80	5	2	80	5
24	62-75-9M	Methanamine, N-methyl-N-nitroso- and others	74.1	153							10	95	20	10	95	20
25	928-45-0	Nitric acid, butyl ester	119.1	136							2	80	5	2	80	5
26	123-75-1	Pyrrolidine	71.1	87	0.60693	0.36363	-0.03004	1.634	0.634	38.80	1	50	2	1	50	2
27	22431-09-	Methanamine, N-(1-methylbutylidene)-	99.2	130							2	80	5	2	80	5
28	616-45-5	2-Pyrrolidinone	85.1	245							10	95	20	10	95	20
29	75-50-3	Methanamine, N,N-dimethyl-	59.1	2.9	-0.09422	0.32583	-0.00337	0.377	0.377	100.00	0	0	1	0	0	1
30	107-12-0	Propanenitrile	55.1	97	0.05925	0.51747	-0.03781	0.319	(0.681)	-213.35	1	50	2	0	0	1
31	109-74-0	Butanenitrile	69.1	118	0.64311	0.38787	-0.03822	1.648	(0.352)	-21.34	2	80	5	1	50	2
32	110-59-8	Pentanenitrile	83.1	139							2	80	5	2	80	5
33	124-12-9	Octanenitrile	125.2	199							10	95	20	10	95	20
34	2243-27-8	Nonanenitrile	139.2	224							10	95	20	10	95	20
35	628-73-9	Hexanenitrile	97.2	162							10	95	20	10	95	20
36	629-08-3	Heptanenitrile	111.2	180							10	95	20	10	95	20
37	75-05-8	Acetonitrile	41.1	81	-0.79666	0.63512	-0.02598	0.035	(0.965)	-2769.19	1	50	2	0	0	1
38	109-21-7	Butanoic acid, butyl ester	144.2	166							10	95	20	10	95	20
39	110-27-0	Tetradecanoic acid, 1-methylethyl ester	270.5	300							40	98	50	40	98	50
40	123-25-1	Butanedioic acid, diethyl ester	174.2	217							40	98	50	40	98	50
41	123-86-4	Acetic acid, butyl ester	116.2	126							2	80	5	2	80	5
42	126-73-8	Phosphoric acid tributyl ester	266.3	289							40	98	50	40	98	50
43	141-78-6	Acetic acid ethyl ester	88.1	77.1	0.63612	0.34441	-0.02691	1.840	0.840	45.65	1	50	2	1	50	2
44	1838-59-1	Formic acid, 2-propenyl ester	86.1	83							1	50	2	1	50	2
45	590-01-2	Propanoic acid, butyl ester	130.2	145							2	80	5	2	80	5
46	591-87-7	Acetic acid, 2-propenyl ester	100.1	103							2	80	5	2	80	5
47	592-84-7	Formic acid, butyl ester	102.1	107							2	80	5	2	80	5
48	84-66-2	1,2-Benzenedicarboxylic acid, diethyl ester	222.2	298							40	98	50	40	98	50
49	1002-84-2	Pentadecanoic acid	242.4	339							40	98	50	40	98	50

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.100			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
					A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
50	107-92-6	Butanoic acid	88.1	163.5	1.22589	0.26481	-0.03737	8.389	(1.611)	-19.20	10	95	20	5	90	10
51	2091-29-4	9-Hexadecenoic acid	254.4	350							40	98	50	40	98	50
52	544-63-8	Tetradecanoic acid	228.4	326							40	98	50	40	98	50
53	57-10-3	Hexadecanoic acid	256.4	399							40	98	50	40	98	50
54	64-19-7	Acetic acid	60.1	118	-0.05553	0.6841	-0.06071	0.158	(1.842)	-1162.90	2	80	5	0	0	1
55	105-42-0	2-Hexanone, 4-methyl-	114.2	140							2	80	5	2	80	5
56	106-35-4	3-Heptanone	114.2	147							2	80	5	2	80	5
57	106-68-3	3-Octanone	128.2	166							10	95	20	10	95	20
58	107-87-9	2-Pentanone	86.1	102							2	80	5	2	80	5
59	108-10-1	2-Pentanone, 4-methyl- (MIBK)	100.2	117.4							2	80	5	2	80	5
60	110-43-0	2-Heptanone	114.2	150							2	80	5	2	80	5
61	111-13-7	2-Octanone	128.2	173							10	95	20	10	95	20
62	112-12-9	2-Undecanone	170.3	229							40	98	50	40	98	50
63	123-19-3	4-Heptanone	114.2	144							2	80	5	2	80	5
64	1534-26-5	3-Tridecanone	198.4	263							40	98	50	40	98	50
65	1534-27-6	3-Dodecanone	184.3	250							40	98	50	40	98	50
66	15932-80-(	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-	152.2	224							40	98	50	40	98	50
67	22026-12-(	6-Tridecanone	198.4	263							40	98	50	40	98	50
68	2216-87-7	3-Undecanone	170.3	227							40	98	50	40	98	50
69	50639-02-(	5-Undecanone, 2-methyl-	184.3	210							40	98	50	40	98	50
70	563-80-4	2-Butanone, 3-methyl-	86.1	94							1	50	2	1	50	2
71	589-38-8	3-Hexanone	100.2	123							2	80	5	2	80	5
72	589-63-9	4-Octanone	128.2	166							10	95	20	10	95	20
73	591-78-6	2-Hexanone	100.2	127							2	80	5	2	80	5
74	593-08-8	2-Tridecanone	198.4	255							40	98	50	40	98	50
75	629-23-2	3-Tetradecanone	212.4	263							40	98	50	40	98	50
76	67-64-1	2-Propanone	58.1	56	-0.14546	0.47497	-0.02286	0.227	(0.773)	-339.84	1	50	2	0	0	1
77	763-93-9	3-Hexen-2-one	98.1	140							2	80	5	2	80	5
78	78-93-3	2-Butanone	72.1	80	0.46525	0.37688	-0.02801	1.149	0.149	12.98	1	50	2	1	50	2
79	78-94-4	3-Buten-2-one	70.1	82							1	50	2	1	50	2
80	821-55-6	2-Nonanone	142.2	195							10	95	20	10	95	20
81	89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)	152.2	224							40	98	50	40	98	50
82	925-78-0	3-Nonanone	142.2	188							10	95	20	10	95	20
83	928-68-7	2-Heptanone, 6-methyl-	128.2	165							10	95	20	10	95	20
84	98-86-2	Ethanone, 1-phenyl-	120.2	201.7							10	95	20	10	95	20
85	110-62-3	Pentanal	86.1	103							2	80	5	2	80	5
86	111-71-7	Heptanal	114.2	153							10	95	20	10	95	20
87	123-38-6	Propanal	58.1	49	0.05519	0.49738	-0.04331	0.327	(0.173)	-52.92	0.5	20	1.25	0	0	1
88	123-72-8	Butanal	72.1	76	0.45056	0.37372	-0.02689	1.122	0.122	10.86	1	50	2	1	50	2
89	124-13-0	Octanal	128.2	171							10	95	20	10	95	20
90	124-19-6	Nonanal	142.2	93							1	50	2	1	50	2
91	19269-28-(	Hexanal, 3-methyl-	114.2	143							2	80	5	2	80	5
92	66-25-1	Hexanal	100.2	131							2	80	5	2	80	5
93	75-07-0	Acetaldehyde	44.1	20.1	-1.17047	0.62766	-0.02475	0.015	0.015	100.00	0	0	1	0	0	1
94	104-76-7	1-Hexanol, 2-ethyl-	130.2	183							10	95	20	10	95	20
95	111-70-6	1-Heptanol	116.2	176							10	95	20	10	95	20
96	112-92-5	1-Octadecanol	270.5	336							40	98	50	40	98	50
97	14898-79-(	2-Butanol	74.1	100	0.76814	0.34611	-0.03478	2.439	1.439	59.00	1	50	2	1	50	2
98	2136-70-1	Ethanol, 2-(tetradecyloxy)-	258.4	253							40	98	50	40	98	50

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.100			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
					A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
99	36653-82-4	1-Hexadecanol	242.4	344							40	98	50	40	98	50
100	51411-24-6	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	224.4	216							40	98	50	40	98	50
101	57-55-6	1,2-Propanediol	76.1	187.6							10	95	20	10	95	20
102	598-32-3	3-Buten-2-ol	72.1	96							1	50	2	1	50	2
103	6032-29-7	2-Pentanol	88.2	118							2	80	5	2	80	5
104	627-27-0	3-Buten-1-ol	72.1	113							2	80	5	2	80	5
105	64-17-5	Ethanol	46.1	78.3	-0.51153	0.67525	-0.04473	0.059	(0.941)	-1604.16	1	50	2	0	0	1
106	67-56-1	Methanol	32.0	64.6	-1.96739	0.82107	-0.01393	0.002	(0.998)	-63343.92	1	50	2	0	0	1
107	67-63-0	2-Propanol	60.1	82.4	0.27183	0.46419	-0.03682	0.590	(0.410)	-69.50	1	50	2	0.5	20	1.25
108	71-23-8	1-Propanol	60.1	97.2	0.38644	0.48033	-0.04505	0.726	(0.274)	-37.70	1	50	2	0.5	20	1.25
109	75-65-0	2-Propanol, 2-methyl-	74.1	82.2							1	50	2	1	50	2
110	75-84-3	1-Propanol, 2,2-dimethyl-	88.2	113							2	80	5	2	80	5
111	75-85-4	2-Butanol, 2-methyl-	88.2	102							2	80	5	2	80	5
112	78-92-2	2-Butanol	74.1	99.5	0.76814	0.34611	-0.03478	2.439	1.439	59.00	1	50	2	1	50	2
113	87-68-3	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	260.8	210							40	98	50	40	98	50
114	96-41-3	Cyclopentanol	86.1	139							2	80	5	2	80	5
115	1184-60-7	1-Propene, 2-fluoro-	60.1	-24							0	0	1	0	0	1
116	127-18-4	Ethene, tetrachloro-	165.8	121.1	1.40596	0.20802	-0.02097	15.030	10.030	66.73	5	90	10	5	90	10
117	156-59-2	Ethene, 1,2-dichloro-, (Z)-	96.9	60	0.47567	0.39061	-0.02554	1.147	0.147	12.81	1	50	2	1	50	2
118	1717-00-6	Ethane, 1,1-dichloro-1-fluoro- (freon 14b)	117.0	32							0.5	20	1.25	0.5	20	1.25
119	56-23-5	Methane, tetrachloro-	153.8	76.7	1.07481	0.28186	-0.02273	5.891	3.891	66.05	2	80	5	2	80	5
120	74-87-3	Methane, chloro- (R-40)	50.5	-24.2	-1.91871	0.62053	-0.00549	0.003	0.003	100.00	0	0	1	0	0	1
121	75-02-5	Ethene, fluoro-	46.0	-72							0	0	1	0	0	1
122	75-09-2	Methane, dichloro-	84.9	39.8	-0.07043	0.4921	-0.02276	0.260	(0.240)	-92.42	0.5	20	1.25	0	0	1
123	75-45-6	Methane, chlorodifluoro- (R-22)	86.5	-40.8							0	0	1	0	0	1
124	75-68-3	Ethane, 1-chloro-1,1-difluoro- (R-142)	100.5	-10							0	0	1	0	0	1
125	75-69-4	Methane, trichlorofluoro- (R-11)	137.4	23.7	0.17307	0.40715	-0.01915	0.558	0.558	100.00	0	0	1	0	0	1
126	6031-02-3	Benzene, (1-methylpentyl)-	162.3	208							40	98	50	40	98	50
127	100-41-4	Benzene, ethyl-	106.2	136.2							2	80	5	2	80	5
128	100-42-5	Benzene, ethenyl-	104.2	145.2							2	80	5	2	80	5
129	106-42-3	Benzene, 1,4-dimethyl-	106.2	138							2	80	5	2	80	5
130	108-38-3	Benzene, 1,3-dimethyl-	106.2	139.1							2	80	5	2	80	5
131	108-88-3	Benzene, methyl-	92.1	110.6							2	80	5	2	80	5
132	3290-53-7	Benzene, (2-methyl-2-propenyl)-	132.2	183							10	95	20	10	95	20
133	538-68-1	Benzene, pentyl-	148.3	205							10	95	20	10	95	20
134	637-50-3	Benzene, 1-propenyl-	118.2	175.5							10	95	20	10	95	20
135	643-58-3	1,1`-Biphenyl, 2-methyl-	168.2	255							40	98	50	40	98	50
136	71-43-2	Benzene	78.1	80.1							1	50	2	1	50	2
137	92-52-4	1,1`-Biphenyl	154.2	255							40	98	50	40	98	50
138	95-47-6	Benzene, 1,2-dimethyl-	106.2	144							2	80	5	2	80	5
139	74-99-7	1-Propyne	40.1	-23	-2.52865	1.74715	-0.21635	0.000	0.000	100.00	0	0	1	0	0	1
140	20184-91-1	4-Nonyne	124.2	154							10	95	20	10	95	20
141	61142-40-3	4-Undecene, 4-methyl-	168.3	193							20	98	50	20	98	50
142	629-73-2	1-Hexadecene	224.4	274							40	98	50	40	98	50
143	74630-39-6	1-Undecene, 4-methyl-	168.3	193							20	98	50	20	98	50
144	74630-48-1	3-Undecene, 2-methyl-, (Z)-	168.3	193							20	98	50	20	98	50
145	764-96-5	5-Undecene, (Z)-	154.3	192.3							20	98	50	20	98	50
146	821-74-9	4,5-Nonadiene	124.2	142.5							2	80	5	2	80	5
147	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	166.3	187							20	98	50	20	98	50

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
					A	B	C	0.100 g ads/100 g carbon			Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out	Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out
148	108-87-2	Cyclohexane, methyl-	98.2	101							2	80	5	2	80	5
149	110-82-7	Cyclohexane	84.2	80.7							1	50	2	1	50	2
150	1472-09-9	Cyclopropane, octyl-	154.3	150.8							20	98	50	20	98	50
151	1618-22-0	Naphthalene, decahydro-2,6-dimethyl-	166.3	187							20	98	50	20	98	50
152	1630-94-0	Cyclopropane, 1,1-dimethyl-	70.1	21							0	0	1	0	0	1
153	1678-93-9	Cyclohexane, butyl-	140.3	181							10	95	20	10	95	20
154	2415-72-7	Cyclopropane, propyl-	84.2	69							1	50	2	1	50	2
155	287-92-3	Cyclopentane	70.1	49.3							0.5	20	1.25	0.5	20	1.25
156	2883-05-8	Octane, 2-cyclohexyl-	196.4	181							20	98	50	20	98	50
157	294-62-2	Cyclododecane	168.3	239							40	98	50	40	98	50
158	2958-76-1	Naphthalene, decahydro-2-methyl-	152.3	201							40	98	50	40	98	50
159	3073-66-3	Cyclohexane, 1,1,3-trimethyl-	126.2	136.6							2	80	5	2	80	5
160	32281-85-1	Cyclopentane, 1,3-dimethyl-2-(1-methylethyl)-	140.3	92							1	50	2	1	50	2
161	3604-14-6	Naphthalene, decahydro-1,2-dimethyl-	166.3	187							20	98	50	20	98	50
162	41977-33-7	Cyclopropane, 1-pentyl-2-propyl-	154.3	151							20	98	50	20	98	50
163	4292-92-6	Cyclohexane, pentyl-	154.3	203.7							40	98	50	40	98	50
164	4806-61-5	Cyclobutane, ethyl-	84.2	71							1	50	2	1	50	2
165	493-02-7	Naphthalene, decahydro-, trans-	138.3	187.3							10	95	20	10	95	20
166	54676-39-0	Cyclohexane, 2-butyl-1,1,3-trimethyl-	182.4	203.7							40	98	50	40	98	50
167	55937-92-3	Bicyclo[4.1.0]heptane, 2-methyl-7-pentyl-	180.3	203.7							40	98	50	40	98	50
168	594-11-6	Cyclopropane, methyl-	56.1	0.7							0	0	1	0	0	1
169	598-61-8	Cyclobutane, methyl-	70.1	36.3							0.5	20	1.25	0.5	20	1.25
170	61142-20-9	Cyclohexane, (4-methylpentyl)-	168.3	203.7							40	98	50	40	98	50
171	7058-01-7	Cyclohexane, (1-methylpropyl)-	140.3	179.3							10	95	20	10	95	20
172	7094-26-0	Cyclohexane, 1,1,2-trimethyl-	126.2	145.2							2	80	5	2	80	5
173	822-50-4	Cyclopentane, 1,2-dimethyl-, trans-	98.2	92							1	50	2	1	50	2
174	1002-43-3	Undecane, 3-methyl-	170.3	195							20	98	50	20	98	50
175	106-97-8	Butane	58.1	-0.45	0.03071	0.34304	-0.01596	0.470	0.470	100.00	0	0	1	0	0	1
176	107-83-5	Pentane, 2-methyl-	86.2	62							1	50	2	1	50	2
177	108-08-7	Pentane, 2,4-dimethyl-	100.2	81							1	50	2	1	50	2
178	109-66-0	Pentane	72.2	36.1							0.5	20	1.25	0.5	20	1.25
179	110-54-3	Hexane	86.2	69							1	50	2	1	50	2
180	111-65-9	Octane	114.2	126							2	80	5	2	80	5
181	111-84-2	Nonane	128.3	150.8							10	95	20	10	95	20
182	1120-21-4	Undecane	156.3	195.6							20	98	50	20	98	50
183	112-40-3	Dodecane	170.3	216.3							40	98	50	40	98	50
184	124-18-5	Decane	142.3	174.1							10	95	20	10	95	20
185	13151-34-3	Decane, 3-methyl-	156.3	190							20	98	50	20	98	50
186	13151-35-4	Decane, 5-methyl-	156.3	190							20	98	50	20	98	50
187	13286-73-2	Tridecane, 3-ethyl-	212.4	252							40	98	50	40	98	50
188	13287-21-3	Tridecane, 6-methyl-	198.4	235							40	98	50	40	98	50
189	142-82-5	Heptane	100.2	98.4							1	50	2	1	50	2
190	14720-74-2	Heptane, 2,2,4-trimethyl-	142.3	148							2	80	5	2	80	5
191	1560-96-9	Tridecane, 2-methyl-	198.4	248							40	98	50	40	98	50
192	1632-70-8	Undecane, 5-methyl-	170.3	195							20	98	50	20	98	50
193	17301-23-4	Undecane, 2,6-dimethyl-	184.4	195							20	98	50	20	98	50
194	17301-25-6	Undecane, 2,8-dimethyl-	184.4	195							20	98	50	20	98	50
195	17301-27-8	Undecane, 2,10-dimethyl-	184.4	195							20	98	50	20	98	50
196	17301-29-0	Undecane, 3,7-dimethyl-	184.4	195							20	98	50	20	98	50

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
					A	B	C	0.100 g ads/100 g carbon			Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out	Estimated Carbon Capacity g/100 g C	Predicted RE %	DF mass in / mass out
197	17301-30-3	Undecane, 3,8-dimethyl-	184.4	195							20	98	50	20	98	50
198	17301-32-4	Undecane, 4,7-dimethyl-	184.4	195							20	98	50	20	98	50
199	17301-94-9	Nonane, 4-methyl-	142.3	165.7							10	95	20	10	95	20
200	17302-28-2	Nonane, 2,6-dimethyl-	156.3	165							20	98	50	20	98	50
201	17302-32-6	Nonane, 3,7-dimethyl-	156.3	165							20	98	50	20	98	50
202	17312-50-4	Decane, 2,5-dimethyl-	170.3	195							20	98	50	20	98	50
203	17312-57-1	Dodecane, 3-methyl-	184.4	216							40	98	50	40	98	50
204	17312-60-6	Undecane, 6-ethyl-	184.4	216							40	98	50	40	98	50
205	17312-73-1	Undecane, 5,5-dimethyl-	184.4	216							40	98	50	40	98	50
206	17312-76-4	Undecane, 6,6-dimethyl-	184.4	216							40	98	50	40	98	50
207	17312-77-5	Undecane, 2,3-dimethyl-	184.4	216							40	98	50	40	98	50
208	17312-80-0	Undecane, 2,4-dimethyl-	184.4	216							40	98	50	40	98	50
209	17312-82-2	Undecane, 4,6-dimethyl-	184.4	216							40	98	50	40	98	50
210	17453-94-0	Undecane, 5-ethyl-	184.4	216							40	98	50	40	98	50
211	20278-85-1	Heptane, 2,3,5-trimethyl-	142.3	160.7							10	95	20	10	95	20
212	2213-23-2	Heptane, 2,4-dimethyl-	128.3	133							2	80	5	2	80	5
213	2216-33-3	Octane, 3-methyl-	128.3	144							2	80	5	2	80	5
214	2216-34-4	Octane, 4-methyl-	128.3	142							2	80	5	2	80	5
215	25117-24-1	Tetradecane, 4-methyl-	212.4	253.7							40	98	50	40	98	50
216	25117-31-1	Tridecane, 5-methyl-	198.4	235							40	98	50	40	98	50
217	26730-12-1	Tridecane, 4-methyl-	198.4	235							40	98	50	40	98	50
218	26730-14-3	Tridecane, 7-methyl-	198.4	235							40	98	50	40	98	50
219	2847-72-5	Decane, 4-methyl-	156.3	187							20	98	50	20	98	50
220	2980-69-0	Undecane, 4-methyl-	170.3	210							40	98	50	40	98	50
221	31295-56-4	Dodecane, 2,6,11-trimethyl-	212.4	252							40	98	50	40	98	50
222	3891-98-3	Dodecane, 2,6,10-trimethyl-	212.4	252							40	98	50	40	98	50
223	4032-93-3	Heptane, 2,3,6-trimethyl-	142.3	156							10	95	20	10	95	20
224	52896-90-9	Heptane, 3-ethyl-5-methyl-	142.3	158.2							10	95	20	10	95	20
225	544-76-3	Hexadecane	226.4	287							40	98	50	40	98	50
226	55030-62-1	Tridecane, 4,8-dimethyl-	212.4	253.7							40	98	50	40	98	50
227	55045-07-3	Dodecane, 2-methyl-8-propyl-	226.4	253.7							40	98	50	40	98	50
228	55045-11-9	Tridecane, 5-propyl-	226.4	253.7							40	98	50	40	98	50
229	562-49-2	Pentane, 3,3-dimethyl-	100.2	90							1	50	2	1	50	2
230	56292-65-0	Dodecane, 2,5-dimethyl-	198.4	235							40	98	50	40	98	50
231	565-59-3	Pentane, 2,3-dimethyl-	100.2	90							1	50	2	1	50	2
232	589-34-4	Hexane, 3-methyl-	100.2	92							1	50	2	1	50	2
233	589-43-5	Hexane, 2,4-dimethyl-	114.2	109							2	80	5	2	80	5
234	589-53-7	Heptane, 4-methyl-	114.2	118							2	80	5	2	80	5
235	589-81-1	Heptane, 3-methyl-	114.2	119							2	80	5	2	80	5
236	591-76-4	Hexane, 2-methyl-	100.2	90							1	50	2	1	50	2
237	592-27-8	Heptane, 2-methyl-	114.2	118							2	80	5	2	80	5
238	61141-72-8	Dodecane, 4,6-dimethyl-	198.4	235							40	98	50	40	98	50
239	6117-97-1	Dodecane, 4-methyl-	184.4	216							40	98	50	40	98	50
240	617-78-7	3-Ethylpentane	100.2	93							1	50	2	1	50	2
241	62016-30-3	Octane, 2,3,3-trimethyl-	156.3	174							20	98	50	20	98	50
242	62016-34-6	Octane, 2,3,7-trimethyl-	156.3	174							20	98	50	20	98	50
243	62108-21-8	Decane, 6-ethyl-2-methyl-	184.4	216							40	98	50	40	98	50
244	62108-25-2	Decane, 2,6,7-trimethyl-	184.4	216							40	98	50	40	98	50
245	62108-27-4	Decane, 2,4,6-trimethyl-	184.4	216							40	98	50	40	98	50

Table 3-2 Compounds detected >0.1 ppm

no of compound	CAS	Compound Name (COPC)	MW	Boiling pt.	carbon loading estimate constants			assumed outlet equilibrium of isotherm PPMV (y)	difference with BP and MW estimation	% error with Yaws prediction	estimated by BP and MW as per A. Shepherd (Shepherd 2001)			estimated by BP and MW with conservativatism for mixing and values no higher than predicted by Yaws (Yaws 1995)		
								0.100			Estimated Carbon Capacity	Predicted RE	DF	Estimated Carbon Capacity	Predicted RE	DF
					A	B	C	g ads/100 g carbon			g/100 g C	%	mass in / mass out	g/100 g C	%	mass in / mass out
246	62238-13-5	Decane, 2,3,7-trimethyl-	184.4	216							40	98	50	40	98	50
247	629-50-5	Tridecane	184.4	235.4							40	98	50	40	98	50
248	629-59-4	Tetradecane	198.4	253.7							40	98	50	40	98	50
249	629-62-9	Pentadecane	212.4	270.6							40	98	50	40	98	50
250	629-78-7	Heptadecane	240.5	301.8							40	98	50	40	98	50
251	74-98-6	Propane	44.1	-42	-0.7946	0.49029	-0.02398	0.049	0.049	100.00	0	0	1	0	0	1
252	75-28-5	Propane, 2-methyl-	58.1	-11.7	-0.01676	0.33495	-0.01274	0.432	0.432	100.00	0	0	1	0	0	1
253	78-78-4	Butane, 2-methyl-	72.2	30							0.5	20	1.25	0.5	20	1.25
254	96-14-0	Pentane, 3-methyl-	86.2	64							1	50	2	1	50	2
255	565-75-3	Pentane, trimethyl-, isomer	114.3	113.5							2	80	5	2	80	5

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Attachment 4 Tables of DF Analysis Results

Table 4-1 COPCs
Table 4-2 Compounds Detected >0.1 ppmv

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Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
1	100-00-5	p-Nitrochlorobenzene	10000	50	5	50000
2	100-21-0	p-Phthalic acid	20	50	50	1000
3	100-41-4	Ethyl benzene	10000	5	1	10000
4	100-42-5	Styrene	10000	5	1	10000
5	10061-01-5	cis-1,3-Dichloropropene	100	5	1	100
6	10061-02-6	trans-1,3-Dichloropropene	50	5	1	50
7	101-55-3	4-Bromophenylphenyl ether	3.33	50	50	167
8	101-84-8	Diphenyl ether	50	50	5	250
9	106-35-4	3-Heptanone	10000	5	1	10000
10	106-42-3	p-Xylene (Dimethyl benzene)	1000	5	1	1000
11	106-46-7	1,4-Dichlorobenzene	50	20	2	100
12	106-88-7	1,2-Epoxybutane	10000	1.25	1	10000
13	106-93-4	Ethylene dibromide (Dibromoethane)	1	10	10	10
14	106-97-8	Butane (R-600)	10000	1	1	10000
15	106-99-0	1,3-Butadiene	10000	1	1	10000
16	107-02-8	Acrolein	10000	1	1	10000
17	107-05-1	3-Chloropropene (Allyl chloride)	10000	1.25	1	10000
18	107-06-2	1,2-Dichloroethane (Ethylene chloride) (freon 150)	10000	2	1	10000
19	107-12-0	Propionitrile	10000	1	1	10000
20	107-13-1	Acrylonitrile	10000	1	1	10000
21	107-18-6	2-Propene-1-ol	10000	1.25	1	10000
22	107-31-3	Formic acid, methyl ester	10000	1	1	10000
23	107-66-4	Dibutylphosphate	10000	5	1	10000
24	107-87-9	2-Pentanone	10000	5	1	10000
25	108-03-2	1-Nitropropane	10000	5	1	10000
26	108-05-4	Vinyl acetate	10000	2	1	10000
27	108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	10000	5	1	10000
28	108-20-3	Bis(isopropyl)ether	10000	2	1	10000
29	108-38-3	m-Xylene (Dimethyl benzene)	1000	5	1	1000
30	108-39-4	m-Cresol	1000	20	2	2000
31	108-87-2	Methylcyclohexane	10000	5	1	10000
32	108-88-3	Toluene	10000	5	1	10000
33	108-90-7	Chlorobenzene	20	5	5	100
34	108-93-0	Cyclohexanol	10000	20	2	20000
35	108-94-1	Cyclohexanone	10000	20	2	20000
36	108-95-2	Phenol	10	20	20	200
37	109-66-0	n-Pentane	10000	1.25	1	10000
38	109-99-9	Tetrahydrofuran	10000	1.25	1	10000

Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
39	110-12-3	5-Methyl-2-hexanone	10000	5	1	10000
40	110-43-0	2-Heptanone	10000	5	1	10000
41	110-54-3	n-Hexane	10000	2	1	10000
42	110-62-3	n-Valeraldehyde	10000	5	1	10000
43	110-82-7	Cyclohexane	10000	2	1	10000
44	110-83-8	Cyclohexene	10000	2	1	10000
45	110-86-1	Pyridine	10000	5	1	10000
46	111-65-9	n-Octane	10000	5	1	10000
47	111-76-2	Ethylene glycol monobutyl ether	10000	20	2	20000
48	111-84-2	n-Nonane	10000	20	2	20000
49	117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	10000	50	5	50000
50	117-84-0	n-Dioctyl phthalate	10000	50	5	50000
51	120-12-7	Anthracene	1000	50	5	5000
52	120-82-1	1,2,4-Trichlorobenzene	100	50	5	500
53	120-83-2	2,4-Dichlorophenol	3.33	50	50	167
54	121-44-8	Triethylamine	10000	2	1	10000
55	121-69-7	Dimethylaniline	10000	20	2	20000
56	122-39-4	N,N-Diphenylamine	50	50	5	250
57	123-19-3	4-Heptanone	10000	5	1	10000
58	123-38-6	n-Propionaldehyde	10000	1	1	10000
59	123-51-3	3-Methyl-1-butanol	10000	5	1	10000
60	123-86-4	Acetic acid n-butyl ester	10000	5	1	10000
61	123-91-1	1,4-Dioxane	10000	2	1	10000
62	126-73-8	Tributyl phosphate	10000	50	5	50000
63	126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	10000	2	1	10000
64	127-18-4	Perchloroethylene (tetrachloroethylene)	1	10	10	10
65	127-19-5	N,N-Dimethylacetamide	10000	10	1	10000
66	128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	10000	50	5	50000
67	129-00-0	Pyrene	3.33	50	50	167
68	1321-64-8	Pentachloronaphthalene	3.33	50	50	167
69	1321-65-9	Trichloronaphthalene	3.33	50	50	167
70	132-64-9	Dibenzofuran	3.33	50	50	167
71	1335-87-1	Hexachloronaphthalene	3.33	50	50	167
72	1335-88-2	Tetrachloronaphthalene	3.33	50	50	167
73	1336-36-3	Polychlorinated biphenyls (PCBs)	3.33	50	50	167
74	141-78-6	Acetic acid ethyl ester (Ethyl acetate)	10000	2	1	10000
75	141-79-7	4-Methyl-3-penten-2-one	10000	5	1	10000
76	142-82-5	n-Heptane	10000	2	1	10000

Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
77	144-62-7	Oxalic acid	10	20	20	200
78	156-60-5	trans-1,2-Dichloroethylene	10000	1.25	1	10000
79	1634-04-4	Methyl tert-butyl ether	10000	2	1	10000
80	189-55-9	Dibenzo[a,i]pyrene	3.33	50	50	167
81	189-64-0	Dibenzo[a,h]pyrene	3.33	50	50	167
82	191-24-2	Benzo(g,h,i)perylene	3.33	50	50	167
83	191-30-0	Benzo[a,i]pyrene	3.33	50	50	167
84	192-65-4	Dibenzo[a,e]pyrene	3.33	50	50	167
85	193-39-5	Indeno(1,2,3-cd)pyrene	3.33	50	50	167
86	206-44-0	Fluoranthene	3.33	50	50	167
87	208-96-8	Acenaphthylene	3.33	50	50	167
88	2234-13-1	Octachloronaphthalene	3.33	50	50	167
89	224-42-0	Dibenz[a,j]acridine	3.33	50	50	167
90	226-36-8	Dibenz[a,h]acridine	3.33	50	50	167
91	25551-13-7	Trimethyl benzene	1000	20	2	2000
92	26140-60-3	Terphenyls	3.33	50	50	167
93	27154-33-2	Trichlorofluoroethane	1	10	10	10
94	287-92-3	Cyclopentane	10000	1.25	1	10000
95	3697-24-3	5-Methylchrysene	3.33	50	50	167
96	3825-26-1	Ammonium perfluorooctanoate	3.33	50	50	167
97	4170-30-3	2-Butenaldehyde (2-Butenal)	10000	2	1	10000
98	50-00-0	Formaldehyde	10000	1	1	10000
99	50-32-8	Benzo(a)pyrene	3.33	50	50	167
100	53-70-3	Dibenzo(a,h)anthracene	3.33	50	50	167
101	540-59-0	1,2-Dichloroethylene	10000	1.25	1	10000
102	540-84-1	2,2,4-Trimethylpentane	10000	2	1	10000
103	541-73-1	1,3-Dichlorobenzene	50	20	2	100
104	56-23-5	Carbon tetrachloride (R-10)	1	5	5	5
105	563-80-4	3-Methyl-2-butanone	10000	2	1	10000
106	56-49-5	3-Methylcholanthrene	3.33	50	50	167
107	57-14-7	1,1-Dimethylhydrazine	10000	2	1	10000
108	58-90-2	2,3,4,6-Tetrachlorophenol	3.33	10	10	33
109	591-78-6	2-Hexanone	1000	5	1	1000
110	59-50-7	4-Chloro-3-methylphenol	3.33	20	20	67
111	59-89-2	N-Nitrosomorpholine	10000	20	2	20000
112	602-87-9	5-Nitroacenaphthene	3.33	50	50	167
113	60-29-7	Ethyl ether	10000	1.25	1	10000
114	603-34-9	Triphenylamine	3.33	50	50	167
115	60-34-4	Methylhydrazine	10000	1	1	10000
116	60-35-5	Acetamide	10000	20	2	20000

Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
117	621-64-7	Di-n-Propylnitrosamine	10000	20	2	20000
118	624-83-9	Methyl isocyanate	1000	1	1	1000
119	627-13-4	Nitric acid, propyl ester	10000	5	1	10000
120	62-75-9	N-Nitroso-N,N-dimethylamine	10000	20	2	20000
121	630-20-6	1,1,1,2-Tetrachloroethane	1	10	10	10
122	64-17-5	Ethyl alcohol	10000	1	1	10000
123	64-18-6	Formic acid	10000	1	1	10000
124	64-19-7	Acetic acid	10000	1	1	10000
125	67-56-1	Methyl alcohol (Methanol)	10000	1	1	10000
126	67-63-0	2-Propyl alcohol (Isopropanol)	10000	1.25	1	10000
127	67-64-1	2-Propanone (Acetone)	10000	1	1	10000
128	67-66-3	Chloroform (R-20)	1	2	2	2
129	67-72-1	Hexachloroethane	1	50	50	50
130	684-16-2	Hexafluoroacetone	1	1	1	1
131	71-23-8	n-Propyl alcohol	10000	1.25	1	10000
132	71-36-3	n-Butyl alcohol	10000	5	1	10000
133	71-43-2	Benzene	100	2	1	100
134	71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	1000	2	1	1000
135	74-83-9	Bromomethane (Methyl bromide) (halon 1001)	1000	1	1	1000
136	74-87-3	Chloromethane (Methyl chloride) (R-40)	20	1	1	20
137	74-97-5	Bromochloromethane (halon 1011)	1	2	2	2
138	74-99-7	Methylacetylene	10000	1	1	10000
139	75-00-3	Chloroethane	1000	1	1	1000
140	75-01-4	Vinyl chloride (1-Chloroethene)	10000	1	1	10000
141	75-05-8	Acetonitrile	1000	1	1	1000
142	75-07-0	Acetaldehyde	10000	1	1	10000
143	75-09-2	Dichloromethane (Methylene chloride) (R-30)	50	1	1	50
144	75-12-7	Formamide	10000	1	1	10000
145	75-15-0	Carbon disulfide	10000	1.25	1	10000
146	75-21-8	Ethylene oxide (Oxirane)	10000	1	1	10000
147	75-27-4	Bromodichloromethane	1	5	5	5
148	75-34-3	1,1-Dichloroethane	10000	2	1	10000
149	75-35-4	1,1-Dichloroethene (Vinylidene chloride)	10000	1.25	1	10000
150	75-43-4	Dichlorofluoromethane (R-21)	1000	1	1	1000
151	75-45-6	Chlorodifluoromethane (R-22)	50	1	1	50
152	75-50-3	Trimethylamine	10000	1	1	10000

Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
153	75-52-5	Nitromethane	10000	1	1	10000
154	75-55-8	2-Methylaziridine	10000	1	1	10000
155	75-61-6	Difluorodibromomethane (freon 12B2-halon 1202)	1	1	1	1
156	75-63-8	Trifluorobromomethane (R-13B1)	1	1	1	1
157	75-65-0	2-Methyl-2-propanol	10000	2	1	10000
158	75-69-4	Trichlorofluoromethane (R-11)	1	1	1	1
159	75-71-8	Dichlorodifluoromethane (R-12)	1	1	1	1
160	76-03-9	Trichloroacetic acid	1	50	50	50
161	76-11-9	1,1,1,2-Tetrachloro-2,2-difluoroethane (R-112a)	20	5	5	100
162	76-12-0	1,1,2,2-Tetrachloro-1,2-difluoroethane (R-112)	20	5	5	100
163	76-13-1	1,2,2-Trichloro-1,1,2-trifluoroethane (Freon 113)	20	2	2	40
164	76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane (R-114)	1	1	1	1
165	76-15-3	Chloropentafluoroethane (R-115)	1	1	1	1
166	78-83-1	2-Methylpropyl alcohol (Isobutyl alcohol)	10000	5	1	10000
167	78-87-5	1,2-Dichloropropane	1000	2	1	1000
168	78-92-2	1-Methylpropyl alcohol (2-Butanol)	10000	2	1	10000
169	78-93-3	Methyl ethyl ketone (MEK, 2-Butanone)	1000	2	1	1000
170	79-00-5	1,1,2-Trichloroethane	10000	5	1	10000
171	79-01-6	Trichloroethylene	10000	2	1	10000
172	79-09-4	Propionic acid	10000	2	1	10000
173	79-10-7	2-Propenoic acid	10000	2	1	10000
174	79-20-9	Methyl acetate	10000	1	1	10000
175	79-34-5	1,1,2,2-Tetrachloroethane	1	10	10	10
176	83-32-9	Acenaphthene	3.33	50	50	167
177	84-66-2	Diethyl phthalate	10000	50	5	50000
178	84-74-2	Dibutyl phthalate	10000	50	5	50000
179	85-01-8	Phenanthrene	3.33	50	50	167
180	85-68-7	Butylbenzyl phthalate	10000	50	5	50000
181	86-73-7	Fluorene	3.33	50	50	167
182	87-68-3	Hexachlorobutadiene	50	50	5	250
183	88-06-2	2,4,6-Trichlorophenol	3.33	50	50	167
184	88-72-2	2-Nitrotoluene	10000	20	2	20000
185	88-75-5	2-Nitrophenol	3.33	20	20	67
186	88-89-1	Picric acid	10000	50	5	50000
187	91-20-3	Naphthalene	100	20	2	200

Table 4-1 COPCs

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
188	91-22-5	Quinoline	10000	20	2	20000
189	91-58-7	2-Chloronapthalene	3.33	50	50	167
190	92-52-4	1,1`-Biphenyl	1000	50	5	5000
191	92-93-3	4-Nitrobiphenyl	3.33	50	50	167
192	95-13-6	Indene	1000	20	2	2000
193	95-47-6	o-Xylene	10000	5	1	10000
194	95-48-7	o-Cresol (2-Methylphenol)	1000	20	2	2000
195	95-49-8	2-Chlorotoluene	10000	20	2	20000
196	95-50-1	o-Dichlorobenzene (1,2-Dichlorobenzene)	50	20	2	100
197	95-57-8	2-Chlorophenol	10000	20	2	20000
198	95-95-4	2,4,5-Trichlorophenol	3.33	50	50	167
199	96-18-4	1,2,3-Trichloropropane	10000	20	2	20000
200	96-22-0	3-Pentanone	10000	5	1	10000
201	96-69-5	Bis(3-tert-butyl-4-hydroxy-6-methyl-phenyl)sulfide	3.33	50	50	167
202	98-51-1	p-tert-Butyltoluene	10000	20	2	20000
203	98-82-8	Cumene	10000	20	2	20000
204	98-83-9	alpha-Methylstyrene	100	20	2	200
205	98-86-2	Acetophenone	100	20	2	200
206	98-95-3	Nitrobenzene	10000	20	2	20000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
1	541-05-9	Cyclotrisiloxane, hexamethyl-	10000	10	1	10000
2	556-67-2	Cyclotetrasiloxane, octamethyl-	10000	50	5	50000
3	USI000-06	tetramethylcyclotrisiloxane	10000	10	1	10000
4	3622-84-2	Benzenesulfonamide, N-butyl-	5	50	50	250
5	5145-07-1	2(3H)-Furanone, dihydro-3,5-dimethyl-	10000	20	2	20000
6	108-47-4	Pyridine, 2,4-dimethyl-	10000	20	2	20000
7	109-99-9	Furan, tetrahydro-	10000	1.25	1	10000
8	110-00-9	Furan	10000	1	1	10000
9	110-86-1	Pyridine	10000	5	1	10000
10	1708-29-8	Furan, 2,5-dihydro-	10000	1.25	1	10000
11	24405-16-1	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	10000	20	2	20000
12	289-95-2	Pyrimidine	10000	5	1	10000
13	290-37-9	Pyrazine	10000	5	1	10000
14	534-22-5	Furan, 2-methyl-	10000	2	1	10000
15	930-22-3	Oxirane, ethenyl-	10000	2	1	10000
16	96-48-0	2(3H)-Furanone, dihydro- (gamma butyrolactone)	10000	10	1	10000
17	3457-90-7	1,3-Propanediol, dinitrate	10000	5	1	10000
18	3457-91-8	1,4-Butanediol, dinitrate	10000	10	1	10000
19	544-16-1	Nitrous acid, butyl ester	10000	2	1	10000
20	624-91-9	Nitrous acid, methyl ester	10000	2	1	10000
21	625-58-1	Nitric acid, ethyl ester	10000	2	1	10000
22	627-05-4	Butane, 1-nitro-	10000	20	2	20000
23	627-13-4	Nitric acid, propyl ester	10000	5	1	10000
24	62-75-9M	Methanamine, N-methyl-N-nitroso- and others	10000	20	2	20000
25	928-45-0	Nitric acid, butyl ester	10000	5	1	10000
26	123-75-1	Pyrrolidine	10000	2	1	10000
27	22431-09-0	Methanamine, N-(1-methylbutylidene)-	10000	5	1	10000
28	616-45-5	2-Pyrrolidinone	10000	20	2	20000
29	75-50-3	Methanamine, N,N-dimethyl-	10000	1	1	10000
30	107-12-0	Propanenitrile	10000	1	1	10000
31	109-74-0	Butanenitrile	10000	2	1	10000
32	110-59-8	Pentanenitrile	10000	5	1	10000
33	124-12-9	Octanenitrile	10000	20	2	20000
34	2243-27-8	Nonanenitrile	10000	20	2	20000
35	628-73-9	Hexanenitrile	10000	20	2	20000
36	629-08-3	Heptanenitrile	10000	20	2	20000
37	75-05-8	Acetonitrile	1000	1	1	1000
38	109-21-7	Butanoic acid, butyl ester	10000	20	2	20000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
39	110-27-0	Tetradecanoic acid, 1-methylethyl ester	10000	50	5	50000
40	123-25-1	Butanedioic acid, diethyl ester	10000	50	5	50000
41	123-86-4	Acetic acid, butyl ester	10000	5	1	10000
42	126-73-8	Phosphoric acid tributyl ester	10000	50	5	50000
43	141-78-6	Acetic acid ethyl ester	10000	2	1	10000
44	1838-59-1	Formic acid, 2-propenyl ester	10000	2	1	10000
45	590-01-2	Propanoic acid, butyl ester	10000	5	1	10000
46	591-87-7	Acetic acid, 2-propenyl ester	10000	5	1	10000
47	592-84-7	Formic acid, butyl ester	10000	5	1	10000
48	84-66-2	1,2-Benzenedicarboxylic acid, diethyl ester	1000	50	5	5000
49	1002-84-2	Pentadecanoic acid	10000	50	5	50000
50	107-92-6	Butanoic acid	10000	10	1	10000
51	2091-29-4	9-Hexadecenoic acid	10000	50	5	50000
52	544-63-8	Tetradecanoic acid	10000	50	5	50000
53	57-10-3	Hexadecanoic acid	10000	50	5	50000
54	64-19-7	Acetic acid	10000	1	1	10000
55	105-42-0	2-Hexanone, 4-methyl-	10000	5	1	10000
56	106-35-4	3-Heptanone	10000	5	1	10000
57	106-68-3	3-Octanone	1000	20	2	2000
58	107-87-9	2-Pentanone	10000	5	1	10000
59	108-10-1	2-Pentanone, 4-methyl- (MIBK)	10000	5	1	10000
60	110-43-0	2-Heptanone	1000	5	1	1000
61	111-13-7	2-Octanone	1000	20	2	2000
62	112-12-9	2-Undecanone	10000	50	5	50000
63	123-19-3	4-Heptanone	1000	5	1	1000
64	1534-26-5	3-Tridecanone	10000	50	5	50000
65	1534-27-6	3-Dodecanone	10000	50	5	50000
66	15932-80-6	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-	10000	50	5	50000
67	22026-12-6	6-Tridecanone	10000	50	5	50000
68	2216-87-7	3-Undecanone	10000	50	5	50000
69	50639-02-6	5-Undecanone, 2-methyl-	10000	50	5	50000
70	563-80-4	2-Butanone, 3-methyl-	10000	2	1	10000
71	589-38-8	3-Hexanone	1000	5	1	1000
72	589-63-9	4-Octanone	1000	20	2	2000
73	591-78-6	2-Hexanone	1000	5	1	1000
74	593-08-8	2-Tridecanone	10000	50	5	50000
75	629-23-2	3-Tetradecanone	10000	50	5	50000
76	67-64-1	2-Propanone	10000	1	1	10000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
77	763-93-9	3-Hexen-2-one	1000	5	1	1000
78	78-93-3	2-Butanone	1000	2	1	1000
79	78-94-4	3-Buten-2-one	1000	2	1	1000
80	821-55-6	2-Nonanone	10000	20	2	20000
81	89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)	10000	50	5	50000
82	925-78-0	3-Nonanone	10000	20	2	20000
83	928-68-7	2-Heptanone, 6-methyl-	1000	20	2	2000
84	98-86-2	Ethanone, 1-phenyl-	100	20	2	200
85	110-62-3	Pentanal	10000	5	1	10000
86	111-71-7	Heptanal	10000	20	2	20000
87	123-38-6	Propanal	10000	1	1	10000
88	123-72-8	Butanal	10000	2	1	10000
89	124-13-0	Octanal	10000	20	2	20000
90	124-19-6	Nonanal	10000	2	1	10000
91	19269-28-4	Hexanal, 3-methyl-	10000	5	1	10000
92	66-25-1	Hexanal	10000	5	1	10000
93	75-07-0	Acetaldehyde	10000	1	1	10000
94	104-76-7	1-Hexanol, 2-ethyl-	10000	20	2	20000
95	111-70-6	1-Heptanol	10000	20	2	20000
96	112-92-5	1-Octadecanol	10000	50	5	50000
97	14898-79-4	2-Butanol	10000	2	1	10000
98	2136-70-1	Ethanol, 2-(tetradecyloxy)-	10000	50	5	50000
99	36653-82-4	1-Hexadecanol	10000	50	5	50000
100	51411-24-6	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	10000	50	5	50000
101	57-55-6	1,2-Propanediol	10000	20	2	20000
102	598-32-3	3-Buten-2-ol	10000	2	1	10000
103	6032-29-7	2-Pentanol	10000	5	1	10000
104	627-27-0	3-Buten-1-ol	10000	5	1	10000
105	64-17-5	Ethanol	10000	1	1	10000
106	67-56-1	Methanol	10000	1	1	10000
107	67-63-0	2-Propanol	10000	1.25	1	10000
108	71-23-8	1-Propanol	10000	1.25	1	10000
109	75-65-0	2-Propanol, 2-methyl-	10000	2	1	10000
110	75-84-3	1-Propanol, 2,2-dimethyl-	10000	5	1	10000
111	75-85-4	2-Butanol, 2-methyl-	10000	5	1	10000
112	78-92-2	2-Butanol	10000	2	1	10000
113	87-68-3	1,3-Butadiene, 1,1,2,3,4,4-hexachloro-	50	50	5	250
114	96-41-3	Cyclopentanol	10000	5	1	10000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
115	1184-60-7	1-Propene, 2-fluoro-	100	1	1	100
116	127-18-4	Ethene, tetrachloro-	1	10	10	10
117	156-59-2	Ethene, 1,2-dichloro-, (Z)-	10000	2	1	10000
118	1717-00-6	Ethane, 1,1-dichloro-1-fluoro- (freon 14b)	1000	1.25	1	1000
119	56-23-5	Methane, tetrachloro-	1	5	5	5
120	74-87-3	Methane, chloro- (R-40)	20	1	1	20
121	75-02-5	Ethene, fluoro-	10000	1	1	10000
122	75-09-2	Methane, dichloro-	20	1	1	20
123	75-45-6	Methane, chlorodifluoro- (R-22)	50	1	1	50
124	75-68-3	Ethane, 1-chloro-1,1-difluoro- (R-142)	50	1	1	50
125	75-69-4	Methane, trichlorofluoro- (R-11)	1	1	1	1
126	6031-02-3	Benzene, (1-methylpentyl)-	10000	50	5	50000
127	100-41-4	Benzene, ethyl-	10000	5	1	10000
128	100-42-5	Benzene, ethenyl-	10000	5	1	10000
129	106-42-3	Benzene, 1,4-dimethyl-	1000	5	1	1000
130	108-38-3	Benzene, 1,3-dimethyl-	1000	5	1	1000
131	108-88-3	Benzene, methyl-	10000	5	1	10000
132	3290-53-7	Benzene, (2-methyl-2-propenyl)-	10000	20	2	20000
133	538-68-1	Benzene, pentyl-	10000	20	2	20000
134	637-50-3	Benzene, 1-propenyl-	10000	20	2	20000
135	643-58-3	1,1`-Biphenyl, 2-methyl-	10000	50	5	50000
136	71-43-2	Benzene	1000	2	1	1000
137	92-52-4	1,1`-Biphenyl	1000	50	5	5000
138	95-47-6	Benzene, 1,2-dimethyl-	10000	5	1	10000
139	74-99-7	1-Propyne	10000	1	1	10000
140	20184-91-2	4-Nonyne	10000	20	2	20000
141	61142-40-3	4-Undecene, 4-methyl-	10000	50	5	50000
142	629-73-2	1-Hexadecene	10000	50	5	50000
143	74630-39-0	1-Undecene, 4-methyl-	10000	50	5	50000
144	74630-48-1	3-Undecene, 2-methyl-, (Z)-	10000	50	5	50000
145	764-96-5	5-Undecene, (Z)-	10000	50	5	50000
146	821-74-9	4,5-Nonadiene	1000	5	1	1000
147	1008-80-6	Naphthalene, decahydro-2,3-dimethyl-	10000	50	5	50000
148	108-87-2	Cyclohexane, methyl-	10000	5	1	10000
149	110-82-7	Cyclohexane	10000	2	1	10000
150	1472-09-9	Cyclopropane, octyl-	10000	50	5	50000
151	1618-22-0	Naphthalene, decahydro-2,6-dimethyl-	10000	50	5	50000
152	1630-94-0	Cyclopropane, 1,1-dimethyl-	10000	1	1	10000
153	1678-93-9	Cyclohexane, butyl-	10000	20	2	20000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
154	2415-72-7	Cyclopropane, propyl-	10000	2	1	10000
155	287-92-3	Cyclopentane	10000	1.25	1	10000
156	2883-05-8	Octane, 2-cyclohexyl-	10000	50	5	50000
157	294-62-2	Cyclododecane	10000	50	5	50000
158	2958-76-1	Naphthalene, decahydro-2-methyl-	10000	50	5	50000
159	3073-66-3	Cyclohexane, 1,1,3-trimethyl-	10000	5	1	10000
160	32281-85-9	Cyclopentane, 1,3-dimethyl-2-(1-methylethyl)-	10000	2	1	10000
161	3604-14-6	Naphthalene, decahydro-1,2-dimethyl-	10000	50	5	50000
162	41977-33-7	Cyclopropane, 1-pentyl-2-propyl-	10000	50	5	50000
163	4292-92-6	Cyclohexane, pentyl-	10000	50	5	50000
164	4806-61-5	Cyclobutane, ethyl-	10000	2	1	10000
165	493-02-7	Naphthalene, decahydro-, trans-	10000	20	2	20000
166	54676-39-0	Cyclohexane, 2-butyl-1,1,3-trimethyl-	10000	50	5	50000
167	55937-92-3	Bicyclo[4.1.0]heptane, 2-methyl-7-pentyl-	10000	50	5	50000
168	594-11-6	Cyclopropane, methyl-	10000	1	1	10000
169	598-61-8	Cyclobutane, methyl-	10000	1.25	1	10000
170	61142-20-9	Cyclohexane, (4-methylpentyl)-	10000	50	5	50000
171	7058-01-7	Cyclohexane, (1-methylpropyl)-	10000	20	2	20000
172	7094-26-0	Cyclohexane, 1,1,2-trimethyl-	10000	5	1	10000
173	822-50-4	Cyclopentane, 1,2-dimethyl-, trans-	10000	2	1	10000
174	1002-43-3	Undecane, 3-methyl-	10000	50	5	50000
175	106-97-8	Butane	10000	1	1	10000
176	107-83-5	Pentane, 2-methyl-	10000	2	1	10000
177	108-08-7	Pentane, 2,4-dimethyl-	10000	2	1	10000
178	109-66-0	Pentane	10000	1.25	1	10000
179	110-54-3	Hexane	10000	2	1	10000
180	111-65-9	Octane	10000	5	1	10000
181	111-84-2	Nonane	10000	20	2	20000
182	1120-21-4	Undecane	10000	50	5	50000
183	112-40-3	Dodecane	10000	50	5	50000
184	124-18-5	Decane	10000	20	2	20000
185	13151-34-3	Decane, 3-methyl-	10000	50	5	50000
186	13151-35-4	Decane, 5-methyl-	10000	50	5	50000
187	13286-73-2	Tridecane, 3-ethyl-	10000	50	5	50000
188	13287-21-3	Tridecane, 6-methyl-	10000	50	5	50000
189	142-82-5	Heptane	10000	2	1	10000
190	14720-74-2	Heptane, 2,2,4-trimethyl-	10000	5	1	10000
191	1560-96-9	Tridecane, 2-methyl-	10000	50	5	50000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
192	1632-70-8	Undecane, 5-methyl-	10000	50	5	50000
193	17301-23-4	Undecane, 2,6-dimethyl-	10000	50	5	50000
194	17301-25-6	Undecane, 2,8-dimethyl-	10000	50	5	50000
195	17301-27-8	Undecane, 2,10-dimethyl-	10000	50	5	50000
196	17301-29-0	Undecane, 3,7-dimethyl-	10000	50	5	50000
197	17301-30-3	Undecane, 3,8-dimethyl-	10000	50	5	50000
198	17301-32-5	Undecane, 4,7-dimethyl-	10000	50	5	50000
199	17301-94-9	Nonane, 4-methyl-	10000	20	2	20000
200	17302-28-2	Nonane, 2,6-dimethyl-	10000	50	5	50000
201	17302-32-8	Nonane, 3,7-dimethyl-	10000	50	5	50000
202	17312-50-4	Decane, 2,5-dimethyl-	10000	50	5	50000
203	17312-57-1	Dodecane, 3-methyl-	10000	50	5	50000
204	17312-60-6	Undecane, 6-ethyl-	10000	50	5	50000
205	17312-73-1	Undecane, 5,5-dimethyl-	10000	50	5	50000
206	17312-76-4	Undecane, 6,6-dimethyl-	10000	50	5	50000
207	17312-77-5	Undecane, 2,3-dimethyl-	10000	50	5	50000
208	17312-80-0	Undecane, 2,4-dimethyl-	10000	50	5	50000
209	17312-82-2	Undecane, 4,6-dimethyl-	10000	50	5	50000
210	17453-94-0	Undecane, 5-ethyl-	10000	50	5	50000
211	20278-85-7	Heptane, 2,3,5-trimethyl-	10000	20	2	20000
212	2213-23-2	Heptane, 2,4-dimethyl-	10000	5	1	10000
213	2216-33-3	Octane, 3-methyl-	10000	5	1	10000
214	2216-34-4	Octane, 4-methyl-	10000	5	1	10000
215	25117-24-2	Tetradecane, 4-methyl-	10000	50	5	50000
216	25117-31-1	Tridecane, 5-methyl-	10000	50	5	50000
217	26730-12-1	Tridecane, 4-methyl-	10000	50	5	50000
218	26730-14-3	Tridecane, 7-methyl-	10000	50	5	50000
219	2847-72-5	Decane, 4-methyl-	10000	50	5	50000
220	2980-69-0	Undecane, 4-methyl-	10000	50	5	50000
221	31295-56-4	Dodecane, 2,6,11-trimethyl-	10000	50	5	50000
222	3891-98-3	Dodecane, 2,6,10-trimethyl-	10000	50	5	50000
223	4032-93-3	Heptane, 2,3,6-trimethyl-	10000	20	2	20000
224	52896-90-9	Heptane, 3-ethyl-5-methyl-	10000	20	2	20000
225	544-76-3	Hexadecane	10000	50	5	50000
226	55030-62-1	Tridecane, 4,8-dimethyl-	10000	50	5	50000
227	55045-07-3	Dodecane, 2-methyl-8-propyl-	10000	50	5	50000
228	55045-11-9	Tridecane, 5-propyl-	10000	50	5	50000
229	562-49-2	Pentane, 3,3-dimethyl-	10000	2	1	10000
230	56292-65-0	Dodecane, 2,5-dimethyl-	10000	50	5	50000
231	565-59-3	Pentane, 2,3-dimethyl-	10000	2	1	10000

Table 4-2 Compounds Detected >0.1 ppmv

no of compound	CAS #	Compound	Oxidizer DF massflow in / massflow out	Adsorption DF massflow in / massflow out	reduced Adsorption DF massflow in / massflow out	Combined DF massflow in / massflow out
232	589-34-4	Hexane, 3-methyl-	10000	2	1	10000
233	589-43-5	Hexane, 2,4-dimethyl-	10000	5	1	10000
234	589-53-7	Heptane, 4-methyl-	10000	5	1	10000
235	589-81-1	Heptane, 3-methyl-	10000	5	1	10000
236	591-76-4	Hexane, 2-methyl-	10000	2	1	10000
237	592-27-8	Heptane, 2-methyl-	10000	5	1	10000
238	61141-72-8	Dodecane, 4,6-dimethyl-	10000	50	5	50000
239	6117-97-1	Dodecane, 4-methyl-	10000	50	5	50000
240	617-78-7	3-Ethylpentane	10000	2	1	10000
241	62016-30-2	Octane, 2,3,3-trimethyl-	10000	50	5	50000
242	62016-34-6	Octane, 2,3,7-trimethyl-	10000	50	5	50000
243	62108-21-8	Decane, 6-ethyl-2-methyl-	10000	50	5	50000
244	62108-25-2	Decane, 2,6,7-trimethyl-	10000	50	5	50000
245	62108-27-4	Decane, 2,4,6-trimethyl-	10000	50	5	50000
246	62238-13-5	Decane, 2,3,7-trimethyl-	10000	50	5	50000
247	629-50-5	Tridecane	10000	50	5	50000
248	629-59-4	Tetradecane	10000	50	5	50000
249	629-62-9	Pentadecane	10000	50	5	50000
250	629-78-7	Heptadecane	10000	50	5	50000
251	74-98-6	Propane	10000	1	1	10000
252	75-28-5	Propane, 2-methyl-	10000	1	1	10000
253	78-78-4	Butane, 2-methyl-	10000	1.25	1	10000
254	96-14-0	Pentane, 3-methyl-	10000	2	1	10000
255	565-75-3	Pentane, trimethyl-, isomer	10000	5	1	10000

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Attachment 5 Thermal Stability Ranking Study

Figure 9 of Technical Article *Development of a Thermal Stability Based Ranking of Hazardous Organic Compound Incinerability* (Dellinger 2000)

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Table IV. ΔT_{99} as a Function of Waste Feed Concentration (Radical Concentration) for Five Model Compounds[a]

A/A_0	R/R_0	$CHCl_3$	CH_2Cl_2	$C_6H_5CH_3$	CH_3Cl	C_6H_6
1.1	1.02	<−1	<−1	<−1	<−1	−5
1.3	1.06	<−1	<−1	<−1	−2	−14
1.5	1.10	<−1	<−1	−1	−3	−23
2.0	1.20	<−1	<−1	−1	−6	−46
3.0	1.40	<−1	<−1	−3	−12	−88

[a] In this analysis, we have assumed that the additional radical concentration (R/R_0) abstracts a H atom from the model compound at the same rate as a Cl atom. The relationship between waste feed concentration (A/A_0) and radical concentration was determined from a series of equilibrium calculations for nominal incinerability mixtures at 1000 °C.

sumption above 750 °C while H metathesis by OCl and C_2Cl_3 are significant destruction pathways at lower temperatures (*15*).

Effect of Varying Waste Feed Rate and Radical Chains. On the basis of the known complexity of hydrocarbon and chlorinated hydrocarbon reaction systems (*47, 14–17*) it may seem fortuitous that such a simple kinetic model can predict the thermal decomposition behavior of such a wide range of species. We acknowledge the need for detailed chemical kinetic mechanisms to predict the thermal decomposition behavior of a given species over wide ranges of experimental conditions. However, the goal of this kinetic analysis was simply the prediction of T_{99}s for one experimental condition.

Using eq 1, we have iteratively calculated the effect of increases in the waste feed concentration on T_{99} for the five model compounds. As shown in Table IV, results indicate that acceptably small decreases in T_{99} (<20 °C) were observed for all compounds for a factor of 2 increase in waste feed rate and acceptably small decreases were observed for all compounds except benzene for a factor of 3 increase in waste feed concentration (~40% increase in radical concentration). For chloroform and dichloromethane, the insensitivity of T_{99} on waste feed concentration is consistent with mechanisms dominated by molecular elimination reactions. The variance in T_{99} for the other compounds is due to the relative contributions of bimolecular radical attack versus unimolecular reaction.

In principle, radical chain reactions can increase the effect of varying radical concentration. Significant chain lengths ($\lambda > 2$) are not expected under incineration conditions due to termination by the formation of stable H_2 and HCl molecules. Polymerization reactions may have longer chain lengths but these reactions are not likely to contribute to POHC destruction in the H- and Cl-rich environment of an incinerator. Both pseudoequilibrium and kinetic calculations indicate that other readily formed polyatomic radicals (e.g., CH_3, CCl_3) that can participate in short chains are in concentrations lower by a factor of 10–100 than H and Cl. Thus, chain lengths for these species would have to be on the order of 10–100 before they would contribute to POHC destruction, which is highly unlikely. Our calculations indicate that chains of $\lambda \leq 2$ produce shifts in T_{99} of equal or lesser magnitude than the effect of changing the radical concentration of up to a factor of 2.

The above analysis indicates that exceptional compounds that are resistant to unimolecular reaction and exhibit large shifts in T_{99} with small increases in radical concentration do exist (e.g., C_6H_6). However, since the stability of all compounds undergoing bimolecular decomposition will shift in the same direction as the radical concentration is varied, changes in their *relative* T_{99} values

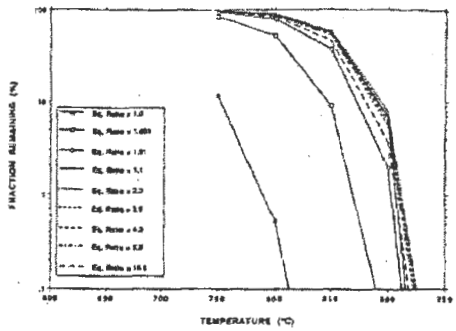

Figure 9. Sensitivity of toluene thermal decomposition behavior as a function of waste/oxygen equivalence ratio. Mixture elemental composition. C_7H_8Cl; t_r = 2.0 s.

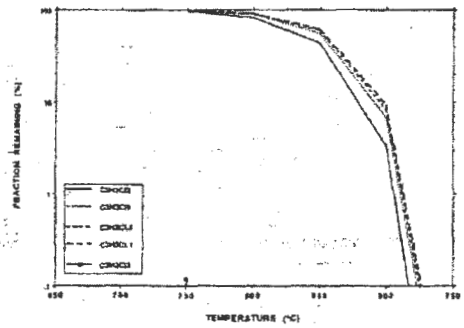

Figure 10. Sensitivity of toluene thermal decomposition behavior as a function of organic mixture Cl atom population. Φ = 3.0; t_r = 2.0 s.

will be suppressed. Since compounds at the top of the ranking decompose predominantly via bimolecular reactions, changes in their relative incinerability are expected to be minimal. Only as we descend through the ranking to where different compounds decompose by bimolecular versus unimolecular pathways will the ranking be expected to exhibit some variance. However, in this regime unimolecular decomposition reactions are available for compounds dominated by bimolecular pathways at nominal conditions. Thus, changes in T_{99} are again expected to be minimal.

Effect of Varying Equivalence Ratio and Waste Feed Composition. Toluene was selected as the model compound for further analysis, as this compound decomposes by numerous bimolecular reactions that are sensitive to changes in reaction atmosphere. We have analyzed the effect of reaction atmosphere by varying the fuel/oxygen stoichiometry ($0.05 < \Phi < 10.0$) for nominal values of mixture elemental composition and by varying mixture elemental composition ($0.33 < H/Cl < 30.0$) for nominal values of fuel/oxygen stoichiometry. Figure 9 presents the results of the sensitivity analysis for variation of waste/oxygen equivalence ratio while Figure 10 presents the results in relation to a variation of Cl and H atom populations, respectively.

Inspection of Figure 9 indicates that for waste/oxygen equivalence ratios ranging from 2.0 to 5.0, there is no significant difference (±10 °C) in T_{99}. As one decreases this parameter to 10.0, a small decrease in T_{99} was ob-

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Attachment 6 VOC Properties and Adsorption Potential

Technology Paper *Activated Carbon Adsorption for Treatment of VOC Emissions* (Shepherd 2001)

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ACTIVATED CARBON ADSORPTION FOR TREATMENT OF VOC EMISSIONS

Presented at the 13th Annual EnviroExpo, Boston Massachusetts—May 2001

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A review of the characteristics of activated carbon and its applicability to emission control of VOC's. Design and costs of carbon systems are also discussed.

INTRODUCTION

The principal use of vapor phase activated carbon in the environmental field is for the removal of volatile organic compounds such as hydrocarbons, solvents, toxic gases and organic based odors. In addition, chemically impregnated activated carbons can be used to control certain inorganic pollutants such as hydrogen sulfide, mercury, or radon.

When properly applied, the adsorption process will remove pollutants for which it is designed, to virtually non-detectable levels. In fact one of the first large- scale uses of activated carbon was in military gas masks where complete contaminant removal is essential. Carbon adsorption is equally effective on single component emissions as well as complex mixtures of pollutants.

In the industrial area, the most common applications of activated carbon are for process off-gases, tank vent emissions, work area air purification, and odor control, either within the plant or related to plant exhausts. Additionally, activated carbon is used in the hazardous waste remediation area to treat off-gases from air strippers and from soil vapor extraction remediation projects.

EVALUATION OF ALTERNATIVE TREATMENT PROCESSES	LOW VOC LEVELS	HIGH VOC LEVELS	CONTINUOS LOADS	INTERMITTENT LOADS	HALOGENATED ORGANICS	TEMP>150F	TEMP<150F	HIGH FLOWS	LOW FLOWS	HIGH HUMIDITY	INORGANIC PARTICLES
ACTIVATED CARBON	•		•	•	•		•	•	•		
THERMALOXIDATION		•	•			•			•	•	
SCRUBBERS	•	•	•			•	•	•	•		
PARTICULATE FILTERS			•	•			•			•	•
CATALYTIC OXIDATION		•	•			•			•	•	

TABLE I

APPLICATION CONSIDERATIONS

One of the major issues that must first be addressed when evaluating a specific environmental VOC problem is what treatment technology to consider. For a given situation there are likely a number of treatment alternatives that appear to have some utility.

The first step in this evaluation is to effectively characterize the application. You will need to know at least the following information:

Flow Rate - Continuos vs intermittent
Contaminants Present – individual contaminants, concentration and variability
Temperature - Average and maximum
Falamibility - Upper and lower explosive limits

Once you have characterized your problem, each technology can be considered for its ability to deal with the conditions identified. As an example, *Table I* lists some of the more common technologies used to control industrial vapor phase pollutants, and the conditions under which they might be most favorably applied. I can't stress enough the importance of this review, as this is where most technical solutions fail. If you solve the wrong problem or pick a technical solution that does not respond to all the variables of your application, poor performance will likely result.

HOW IT WORKS

In the adsorption process, molecules of a contaminated gas are attracted to and accumulate on the surface of the activated carbon. Carbon is a commonly used adsorbent due to its very large surface area. It can be made from a variety of base materials including coal, wood and coconut shells, and is manufactured or activated in a high temperature controlled oxidation process. A pound of highly activated carbon has a surface area approaching 140 acres.

CROSS SECTION OF CARBON

This *Figure I* presents an artist's rendition of the cross section of an activated carbon particle. Note that almost all of the surface area available for adsorption is associated with its internal pore structure. Also note the relative change in pore diameters, going from very large at the granule surface boundary, to much smaller within the particle interior. Balancing of the large and small pore volumes during the activation process is what makes individual activated carbons perform differently. Molecules of a contaminant tend to adsorb most strongly in areas where the pore diameter of the adsorbent is close to the molecular diameter of the compound.

While most organic compounds will adsorb on activated carbon to some degree, the adsorption process is most effective on higher molecular weight and high boiling point compounds.

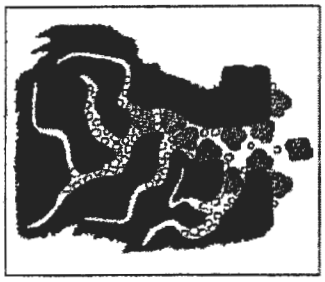


FIGURE I

LIST OF ORGANIC COMPOUNDS

RELATIVE ADSORPTION RATE

		MOLECULAR WEIGHT	BOILING POINT	CARBON CAPACITY %
STRONGER	NITROBENZENE	123	211 C	51
	TETRACHLOROETHANE	166	147 C	40
	TETRACHLOROETHYLENE	165	121 C	35
	STYRENE	104	145 C	25
	XYLENE	106	138 C	21
	NAPATHYLENE	128	217 C	20
	TOLUNE	92	111 C	20
	BENZENE	78	80 C	12
	MTBE	88	55 C	12
	HEXANE	86	68 C	7
	ETHLY ACRILATE	100	57 C	5
	DIDHLOROETHANE	99	99 C	7
	METHYL ETHYLKETONE	72	80 C	4
	METHYLENE CHLORIDE	84	40 C	2
	ACRILONITRILE	53	74 C	2
	ACETONE	58	56 C	0.8
	VINYLCHLORIDE	62	neg 14 C	0.7
	CHLOROETHANE	64	12 C	0.5
	BROMOTRI FLOROMETHANE	149	neg 58 C	0.13
WEAKER	METHANE	16	neg 161 C	0.0003

TABLE II

Compounds having a molecular weight over 50 and a boiling point greater than 50 degrees centigrade are good candidates for adsorption. *TABLE II* presents a representative list of organic compounds and their relative adsorption strength. Organic contaminants are often classified as weakly, moderately, or strongly adsorbed. You will note that a compound such as nitrobenzene having a molecular weight of 123 and a boiling point of 211 C is characterized as a very strong adsorber. On the other hand a compound such as methane which has a molecular weight of 16 and a boiling point of -161 C is a very weakly adsorbed compound. In fact, at this capacity, for all practical purposes, methane removal with activated carbon would not be cost effective.

ABSORPTION CAPACITY

Physical adsorption is dependant on the characteristics of the contaminant to be adsorbed, the temperature of the gas stream to be processed, and the concentration of the contaminant in the gas stream. The adsorption capacity for a particular contaminant represents the amount of the contaminant that can be adsorbed on a unit weight of activated carbon consumed at the conditions present in the application. Typical adsorption capacities for moderately adsorbed compounds range from 5 to 30 percent of the weight of the carbon.

TRICHLOROETHYLENE ISOTHERM

The adsorption isotherm plot shows the influence of concentration on adsorption capacity. *Figure II* presents an adsorption isotherm used to predict adsorption capacity for trichloroethylene. Note how the adsorption capacity varies from 20 to 65 percent over the concentration range of 10 to 10000 ppm in the gas stream.

A series of isotherms at differing temperatures shows the influence of temperature on adsorption capacity. In Figure III you can see the effect of temperature on the same trichloroethylene compound. At 100ppm the capacity of activated carbon for trichloroethylene varies from 17 to 40 percent as the temperature changes from 140 to 32 degrees F.

Fortunately, most carbon suppliers have developed isotherms for a range of environmental contaminants. At Carbtrol we have built a computerized database of adsorption isotherms so that we can easily model most environmental applications. By supplying to us the gas flow rate, the contaminant concentration and the temperature of the gas stream, a carbon usage prediction can be made.

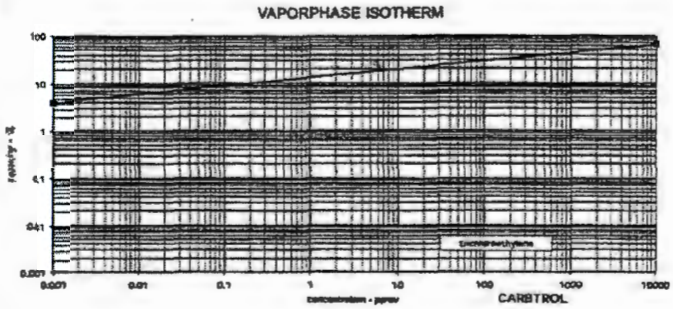


FIGURE II

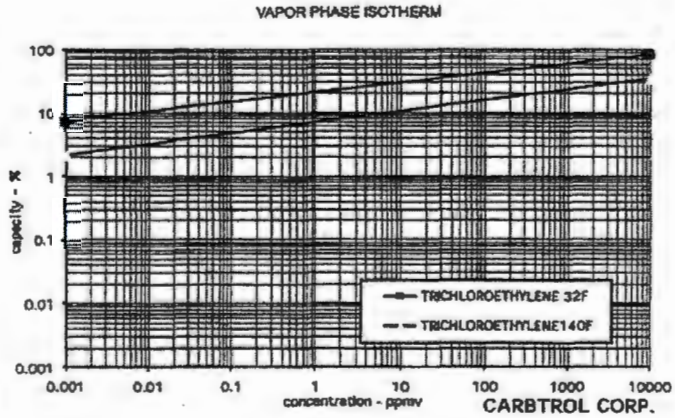
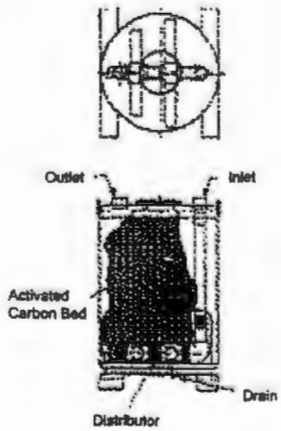


FIGURE III

DESIGN CONSIDERATIONS



CARBTROL G-4 ADSORBER

FIGURE IV

Activated carbons used in the air pollution control field are normally supplied in a granular form with a particle size ranging from 1 to 5 millimeters. In the granular form activated carbon can easily be packed into a containment device through which a contaminated gas stream can be processed for purification.

Figure IV shows the cross section of a typical fixed bed vapor phase adsorber. An adsorption system in its simplest form is made of a containment device (drum or vessel), distribution and collection devices to effect proper circulation of the gas stream through the activated carbon bed, and a means for moving the gas stream through the bed (such as a fan, a blower, or pressurized gas displacement). Packed activated carbon beds can be conveniently config-

ured into small transportable drums or tanks, or into large fixed contacting devices depending on the application.

Adsorber sizing for a particular application is governed primarily by bed surface loading rate. With a standard 4-foot carbon bed depth, a maximum gas-loading rate of 100 cfm per square foot of bed surface should be maintained. This insures adequate gas contact and sufficient time to reach adsorption equilibrium. Higher gas flows are handled by increasing the carbon bed surface (larger adsorbers) or adding multiple beds in parallel.

One of the chief advantages of granular activated carbon adsorption is its simplicity of application. Pre-engineered fixed bed adsorbers can be purchased and installed on most existing exhaust systems with a minimum of capital expenditure. Transportable adsorbers from 100 to 5000 pounds are readily available as standard supply from several manufactures. Air flows for these stock units go up to as much as 5000 CFM. Larger systems up to 20,000 CFM or higher are available on a custom basis. Once installed these systems operate for the most part unattended until the carbon becomes spent and requires replacement. The frequency of replacement will vary for each application but may range from weekly to annually.

Another significant advantage of an adsorption process is that it provides on line reserve capacity on a passive basis. The system is, in effect, available on a continuos basis to handle varying loads but only consumes carbon when contaminants are present in the exhaust stream. Other processes may have significant fuel or chemical operating costs even when no contaminants are being treated.

REACTIVATION

Once the activated carbon has become spent it must be removed from service and replaced with fresh carbon in order to maintain the effectiveness of treatment. The spent carbon can be disposed of and replaced with virgin carbon, or the spent carbon can be returned to the supplier for reactivation and reuse. Reactivation restores most of the original carbon adsorption capacity and avoids expensive disposal costs. Most carbon adsorption applications rely on offsite reactivation to support their activated carbon supply.

The spent carbon can be vacuumed from fixed adsorption vessels and shipped to the reactivation center in bulk, or returned to the reactivation facility in a transportable adsorber that serves both as an adsorption vessel and a UN shipping container.

CAPITAL AND OPERATING COSTS

Adsorption system capital and operating costs can vary widely but depend primarily on the gas volume to be treated and the amount of carbon consumed.

A simple100 cubic foot per minute adsorption system consisting of two 200 pound canisters and a blower would require about 20 sq ft of area and cost about 2-$3,000. When spent these smaller adsorption units can often be exchanged for new units with the original supplier.

Larger custom carbon adsorption systems can cost from several thousand, up to several hundred thousand dollars, and are usually supported with off site reactivation services.

A 5000 cfm system with two adsorbers and an exhaust blower would have a capital cost in the 30-$40,000 range and if skid mounted would take up an area of about 100sq ft.

The Custom reactivation service to support this system usually costs about $2.00 per pound of carbon processed including transportation.

ACTIVATED CARBON QUALITY

You should be aware that there is a significant difference in adsorption capacity among the various commercial activated carbon products available. When procuring activated carbons it is important to recognize that the value of the activated carbon product that you are purchasing is related to its adsorption capacity, and not its weight or volume.

The carbon manufacturing industry, in conjunction with ASTM, has developed several standard tests that enable comparison of the relative adsorption capacities of various activated carbons. These tests can be used to assess the quality of a virgin or reactivated carbon product and to predict its cost effectiveness.

The industry standard quality tests for VAPOR PHASE activated carbons is the CARBON TETRACHLORIDE ADSORPTION CAPACITY, or ASTM D3467. Typical vapor phase virgin activated carbons have CARBON TETRACHLORIDE ADSORPTION CAPACITIES ranging from 45 to 70 percent by weight.

When procuring either virgin or reactivated carbon products, make sure the appropriate adsorption number is specified. Then compare the alternative product specifications to insure you are getting the best activated carbon value.

SUMMARY

In summary, activated carbon has been shown to be applicable for treatment of a wide variety of environmental contaminants. It is a proven technology that is simple to install and easy to operate and maintain. Capital costs are among the least expensive for most alternative treatment technologies. Operating costs are primarily related to the amount of activated carbon consumed in the adsorption process.

Attachment 7 Prediction of VOC Adsorption Capacity

Technical Article *Determining VOC Adsorption Capacity* (Yaws 1995)

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POLLUTION ENGINEERING

Determining VOC Adsorption Capacity

Capacity data for the adsorption of VOCs on activated carbon is needed when meeting stricter air regs.

by Carl L. Yaws, Li Bu and Sachin Nijhawan

Physical and thermodynamic property data for organic compounds are especially helpful to engineers and scientists in industry. In particular, capacity data for adsorption of volatile organic compounds (VOCs) on activated carbon is becoming increasingly important in engineering and environmental studies because of more stringent air emissions regulations.

Results are presented for adsorption capacity as a function of the VOC concentration in the gas. The results can be used in engineering and environmental studies. Capacity data resulting from the correlation are useful in the engineering design of carbon adsorption systems to remove trace pollutants from gases. For pollution control to very low emission levels, such systems could include carbon adsorption followed by conventional steam regeneration with solvent recovery, or carbon adsorption followed by thermal or catalytic oxidation.

Adsorption capacity correlation

The correlation for adsorption on activated carbon is based on a logarithmic series expansion of concentration in the gas:

$$\log_{10}Q = A + B\log_{10}y + C[\log_{10}y]^2$$

where Q = adsorption capacity at equilibrium, g of compound/100 g of carbon

y = concentration in gas at 25°C and 1 atm, parts per million by volume, ppmv

A, B and C = correlation constants

The correlation constants A, B and C in Table 1 were determined from regression of the available data for adsorption on activated carbon. The tabulation is arranged by carbon number (C1, C2, C3...) so data can be quickly located using the chemical formula.

Estimation equation

In preparing the correlation, a literature search was conducted to identify sources for a database of adsorption capacity values at different concentrations (partial pressures). The database also served to check the accuracy of the correlation.

Adsorption capacity for the remaining compounds was then estimated. The following equation (developed by Calgon) was used to estimate the equilibrium adsorption capacity of activated carbon as a fifth order polynomial function of its adsorption potential:

$$\log_{10}Q = A + B\mu + C\mu^2 + D\mu^3 + E\mu^4 + F\mu^5$$

where Q = adsorption capacity at equilibrium, cm_3 of liquid compound/100 g of carbon

μ = adsorption potential of compound, $T/(V_l\Gamma_l)\log(P_l^{sat}/p_l)$

T = temperature, K

V_l = liquid molar volume of compound, cm^3/g-mol

Γ_l = relative polarizability, $[(n^2-1)(n^2+1)]_l/[(n^2-1)(n^2+1)]_{n\text{-hexane}}$

n = refractive index

P_l^{sat} = vapor pressure of compound, atm

p_l = partial pressure of compound, atm

A = 1.71

B = -1.46E-02

C = 1.65E-03

D = -4.11E-04

E = 3.14E-05

F = -6.75E-07

Examples

The correlation may be used to determine adsorption capacity of activated carbon for pollutants.

For example, the air from a paint-spraying operation contains 10 ppmv of n-butanol ($C_4H_{10}O$). The goal is to estimate the adsorption capacity of activated carbon for removing the pollutant at 25° C and 1 atm.

Substitution of the correlation constants from the table and concentration into the correlation equation yields

$$\log_{10}Q = 0.89881 + 0.32534\log_{10}(10) - 0.03648[\log_{10}(10)]^2 = 1.18767$$

Q = 15.41 g of n-butanol/100 g of carbon

In another case the air from an industrial operation contains 100 ppmv of methyl ethyl ketone (C_4H_8O). The adsorption capacity of activated carbon for removing the pollutant at 25° C and 1 atm must be estimated.

Substitution of the correlation constants from the table and concentration into the correlation equation yields

$$\log_{10}Q = 0.46525 + 0.37688\log_{10}(100) - 0.02801[\log_{10}(100)]^2 = 1.10697$$

Q = 12.79 g of methyl ethyl ketone/100 g of carbon

Operation and design

In actual operation under plant conditions, the capacity of an adsorption bed will seldom achieve equilibrium. Air

Table 1. Adsorption on Activated Carbon

No.	Formula	Name	A	B	C	Min	Max	Q @ 10 ppmv	Q @ 100 ppmv	Q @ 1000 ppmv
1	$CBrCl_3$	Bromotrichloromethane	-1.09842	0.23228	-0.02184	10	10000	40.63	59.65	379.20
2	$CBrF_3$	Bromotrifluoromethane	-1.46247	0.58361	-0.01044	10	10000	0.13	0.46	1.56
3	CBr_2F_2	Dibromodifluoromethane	0.82076	0.30701	-0.01384	10	10000	13.00	23.96	41.42
4	CBr_3F	Tribromofluoromethane	-1.43748	0.55503	-0.00450	10	10000	0.13	0.45	1.54
5	CCl_2F_2	Dichlorodifluoromethane	-0.07350	0.40145	-0.01404	10	10000	2.06	4.71	10.10
6	CCl_2O	Phosgene	-0.54469	0.60428	-0.02386	10	10000	0.85	2.78	7.93
7	CCl_3F	Trichlorofluoromethane	0.017307	0.46715	-0.01919	10	10000	3.64	8.14	16.68
8	CCl_3NO_2	Chloropicrin	1.26745	0.20841	-0.01288	10	10000	29.04	42.93	59.81
9	CCl_4	Carbon Tetrachloride	-1.07481	0.73184	-0.01917	10	10000	21.57	35.29	51.98
10	$CHBr_3$	Tribromomethane	0.93184	0.18948	-0.02246	10	723.8	181.07	109.89	34.33
11	$CHCl_3$	Chloroform	0.67102	0.31148	-0.02288	10	10000	10.23	20.07	35.45
12	CHN	Hydrogen Cyanide	-0.19745	0.28948	-0.00740	10	10000	4.9E-04	2E-03	6.4E-02
13	$CHBrCl_2$	Bromochloromethane	0.61399	0.41353	-0.02531	10	10000	10.05	21.87	42.35
14	$CHBrF_2$	Bromofluoromethane	0.45483	0.36332	-0.01606	10	10000	6.34	13.10	25.13
15	CH_2Br_2	Dibromomethane	1.08376	0.37211	-0.03238	10	10000	26.52	49.94	81.04
16	CH_2Cl_2	Dichloromethane	-0.02841	0.49210	-0.02218	10	10000	2.51	6.63	15.89
17	CH_3I	Diiodomethane	1.34756	0.14964	-0.01947	10	1581	119.66	147.70	166.67
18	CH_2O	Formaldehyde	-2.48524	0.69123	-0.00375	10	10000	1.6E-02	7.6E-02	0.36
19	CH_2O_2	Formic Acid	-1.72731	1.09503	-0.06354	10	10000	0.18	1.44	8.63
20	CH_3Br	Methyl Bromide	-1.22435	0.78564	-0.05521	10	10000	0.31	1.29	4.19
21	CH_3Cl	Methyl Chloride	-0.43831	0.63681	-0.06945	10	10000	5.0E-03	0.20	0.28
22	CH_2Cl_2	Methyl Dichloride	0.09198	0.34725	-0.01971	10	10000	159.25	102.74	47.48
23	CH_3I	Methyl Iodide	0.73997	0.32985	-0.01330	10	10000	11.39	22.23	40.72
24	$CHNO$	Formamide	1.30981	0.25174	—	10	80	36.52	—	—
25	CH_3NO_2	Nitromethane	-0.17847	0.70607	-0.05111	10	10000	2.12	7.57	21.36
26	CH_4	Methane	-4.31008	0.77881	-0.00628	10	10000	2.9E-04	1.7E-03	9.3E-03
27	CH_5ClSi	Methyl Dichlorosilane	0.73271	0.29305	-0.01822	10	10000	10.17	17.62	28.04
28	CH_4O	Methanol	-1.96739	0.82107	-0.01989	10	10000	6.9E-02	0.42	2.35
29	CH_4S	Methyl Mercaptan	-1.12288	0.60573	-0.02094	10	10000	0.29	1.01	3.21
30	CH_5N	Methylamine	-1.93548	0.64710	-0.01037	10	10000	5.0E-02	0.21	0.81
31	CN_2O_2	Tetranitromethane	1.49047	0.18181	-0.01894	10	10000	45.01	60.02	73.35
32	CO	Carbon Monoxide	-5.18782	0.90121	-0.01358	10	10000	3.0E-05	3.6E-04	2.5E-03
33	COS	Carbonyl Sulfide	-1.42882	0.51061	0.00028	10	10000	0.12	0.33	1.27
34	CO_2	Carbon Dioxide	-3.53214	0.80180	-0.00328	10	10000	4E-03	1.2E-03	3.1E-02
35	CS_2	Carbon Disulfide	0.18499	0.47093	-0.01481	10	10000	18.25	4.94	12.32
36	$C_2Br_2F_4$	1,2-Dibromotetrafluoroethane	0.90388	0.25693	-0.00974	10	10000	14.16	22.92	38.64
37	C_2ClF_5	Chloropentafluoroethane	0.08264	0.34756	-0.01343	10	10000	2.61	5.30	10.10
38	$C_2Cl_3F_3$	1,1,2-Trichlorotrifluoroethane	1.37368	0.18656	-0.01231	10	10000	28.05	39.59	52.79
39	C_2Cl_4	Tetrachloroethylene	1.83186	0.20802	-0.02097	10	10000	39.17	54.72	69.39
40	$C_2Cl_4F_2$	1,1,2,2-Tetrachlorodifluoroethane	1.37307	0.17625	-0.01465	10	10000	34.25	46.45	58.88
41	$C_2HBrClF_3$	Halothane	0.92405	0.31204	-0.02004	10	10000	16.45	29.38	47.84
42	C_2HCl_3	Trichloroethylene	1.02611	0.29829	-0.02519	10	10000	19.86	33.20	49.38
43	C_2HCl_3O	Trichloroacetyl Chloride	1.8147	0.26219	-0.02596	10	10000	29.70	45.19	61.57
44	C_2HCl_3O	Trichloroacetaldehyde	1.2361	0.25931	-0.02513	10	10000	26.19	40.98	57.09
45	C_2HCl_5	Pentachloroethane	1.4366	0.33515	-0.01572	10	4829	59.22	71.30	81.22
46	$C_2HF_3O_2$	Trifluoroacetic Acid	-0.12577	0.59173	-0.03445	10	10000	2.713	8.39	22.15
47	C_2H_2	Acetylene	-2.24177	0.82454	-0.03390	10	10000	3.5E-02	0.19	0.84
48	$C_2H_2Br_4$	1,1,2,2-Tetrabromoethane	—	—	—	—	—	146.05	—	—
49	$C_2H_2Cl_2$	1,1-Dichloroethylene	0.48740	0.33282	-0.01622	10	10000	6.37	12.25	21.87
50	$C_2H_2Cl_2$	cis-1,2-Dichloroethylene	0.47567	0.39061	-0.02534	10	10000	6.93	14.28	26.18
51	$C_2H_2Cl_2$	trans-1,2-Dichloroethylene	0.47567	0.39061	-0.02534	10	10000	6.93	14.28	26.16
52	$C_2H_2Cl_2O_2$	Dichloroacetic Acid	1.49237	0.09630	—	10	235	61.47	76.73	—
53	$C_2H_2Cl_4$	1,1,1,2-Tetrachloroethane	1.44097	0.19166	-0.01995	10	10000	40.99	55.52	68.61
54	$C_2H_2Cl_4$	1,1,2,2-Tetrachloroethane	1.32322	0.17848	-0.02019	10	6073	48.03	63.01	75.33
55	C_2H_3Cl	Vinyl Chloride	-0.98889	0.66564	-0.04320	10	10000	0.43	1.48	4.16
56	C_2H_3ClO	Acetyl Chloride	0.03527	0.45526	-0.02093	10	10000	2.96	7.30	16.35
57	$C_2H_3ClO_2$	Methyl Chloroformate	0.41186	0.42776	-0.02776	10	10000	6.48	14.33	27.88
58	$C_2H_3Cl_3$	1,1,1-Trichloroethane	0.97331	0.28737	-0.02277	10	10000	17.29	28.64	42.70
59	$C_2H_3Cl_3$	1,1,2-Trichloroethane	1.17161	0.27791	-0.02246	10	10000	26.43	41.46	57.31
60	C_2H_3N	Acetonitrile	-0.18444	0.63612	-0.02598	10	10000	0.65	2.34	7.50
61	C_2H_3NO	Methyl Isocyanate	-1.07579	0.85881	-0.06826	10	10000	0.52	2.33	7.62
62	C_2H_4	Ethylene	-2.27102	0.61731	-0.01467	10	10000	2.1E-02	8.0E-02	0.28
63	$C_2H_4Br_2$	1,1-Dibromoethane	1.37260	0.25671	-0.02516	10	10000	40.19	61.01	82.48
64	$C_2H_4Br_2$	1,2-Dibromoethane	1.44231	0.25500	-0.02666	10	10000	46.84	70.09	92.77
65	$C_2H_4Cl_2$	1,1-Dichloroethane	0.54485	0.36091	-0.02192	10	10000	7.65	15.10	26.93
66	$C_2H_4Cl_2$	1,2-Dichloroethane	0.55343	0.37072	-0.02161	10	10000	7.99	16.16	29.59
67	$C_2H_4Cl_2O$	Bis(chloromethyl)ether	0.95399	0.33784	-0.03200	10	10000	8.27	31.89	48.04
68	$C_2H_4F_2$	1,2-Difluoroethane	-3.97902	-2.51862	-0.31617	10	10000	0.02	0.62	5.39
69	C_2H_4O	Acetaldehyde	-0.42847	0.88788	-0.05275	10	10000	0.27	0.97	3.09
70	C_2H_4O	Ethylene Oxide	-2.42379	0.94478	-0.04062	10	10000	0.03	0.20	1.14
71	$C_2H_4O_2$	Acetic Acid	-0.68683	0.68439	-0.04879	10	10000	3.70	11.74	28.21
72	$C_2H_4O_2$	Methyl Formate	-0.99586	0.61693	-0.01847	10	10000	0.40	1.46	4.88
73	C_2H_4S	Thiacyclopropane	0.62258	0.45520	-0.02154	10	10000	2.86	7.03	15.64
74	C_2H_5Br	Bromoethane	0.31783	0.43549	-0.03072	10	10000	5.28	11.64	22.27
75	C_2H_5Cl	Ethyl Chloride	-0.50478	0.50164	-0.02179	10	10000	0.94	2.58	6.40
76	C_2H_5ClO	2-Chloroethanol	0.74164	0.46933	-0.05138	10	9446	14.43	29.78	48.46
77	C_2H_5I	Ethyl Iodide	1.00356	0.32123	-0.02405	10	10000	19.99	35.47	56.33
78	C_2H_5N	Ethylenimine	-1.16912	0.91238	-0.07400	10	10000	0.47	2.29	7.98
79	C_2H_5NO	N-Methylformamide	1.23333	0.21723	—	10	333	26.22	46.34	—
80	$C_2H_5NO_2$	Nitroethane	0.44968	0.49708	-0.04612	10	10000	7.96	18.17	33.86
81	C_2H_6	Ethane	-2.40393	0.68107	-0.01925	10	10000	1.8E-02	7.6E-02	0.29
82	C_2H_6O	Ethanol	-0.81153	0.69529	-0.04479	10	10000	1.32	4.57	12.83
83	C_2H_6OS	Dimethyl Sulfoxide	1.24042	0.31302	-0.04768	10	802	32.05	47.40	—

[redacted]

Table 1. Adsorption on Activated Carbon

No.	Formula	Name	A	B	C	Min	Max	Q @ 10 ppmv	Q @ 100 ppmv	Q @ 1000 ppmv
84	$C_2H_6O_2$	Ethylene Glycol	1.40474	0.18738	−0.02663	10	121	36.27	47.09	—
85	CH_6O_4S	Dimethyl Sulfate	1.34611	0.21539	−0.02336	10	890	34.53	48.23	—
86	CH_6S	Dimethyl Sulfide	0.48472	0.37358	−0.02770	10	10000	6.77	13.22	22.71
87	CH_4S	Ethyl Mercaptan	0.00552	0.40506	−0.01802	10	10000	2.47	5.54	11.44
88	$C_2H_6S_2$	Dimethyl Disulfide	0.73878	0.35828	−0.02953	10	10000	12.26	22.87	37.23
89	CH_5N	Dimethylamine	−1.22492	0.63962	−0.03266	10	10000	0.24	0.84	2.51
90	CH_7NO	Monoethanolamine	1.21569	0.21994	—	10	485	27.17	45.24	—
91	CH_4N_2	Ethylenediamine	0.56504	0.46307	−0.04789	10	10000	9.55	19.94	33.36
92	C_3H_5Cl	Propargyl Chloride	0.27135	0.40480	−0.02135	10	10000	4.52	9.90	19.66
93	C_3H_3N	Acrylonitrile	0.07669	0.49986	−0.03500	10	10000	3.48	8.64	18.25
94	C_3H_7NO	Oxazole	0.63350	0.30620	−0.02350	10	10000	8.25	14.19	21.91
95	C_3H_4	Methylacetylene	[redacted]			10	10000	0.30	2.26	5.83
96	$C_3H_4Cl_2$	2,3-Dichloropropene	0.95417	0.30034	−0.02674	10	10000	16.92	28.20	47.68
97	C_3H_4O	Acrolein	−0.29632	0.49437	−0.02471	10	10000	1.49	3.92	9.21
98	C_3H_6O	Propargyl Alcohol	0.22971	0.57711	−0.05441	10	10000	5.65	14.67	29.61
99	$C_3H_4O_2$	Acrylic Acid	0.75549	0.47108	−0.05615	10	5221	14.81	29.72	46.06
100	$C_3H_4O_3$	Pyruvic Acid	1.07410	0.41414	−0.05768	10	1679	26.95	46.95	62.72
101	C_3H_5Br	3-Bromo-1-Propene	0.84815	0.32392	−0.02398	10	10000	14.06	25.12	40.19
102	C_3H_5Cl	3-Chloropropene	0.32792	0.36553	−0.01853	10	10000	4.73	9.66	18.10
103	C_3H_5ClO	alpha-Epichlorohydrin	0.83203	0.38983	−0.03932	10	10000	15.22	28.47	44.42
104	$C_3H_5ClO_2$	Methyl Chloroacetate	1.07657	0.32514	−0.03612	10	9959	23.20	38.21	53.27
105	$C_3H_5ClO_2$	Ethyl Chloroformate	0.94901	0.32529	−0.03201	10	10000	17.47	29.62	43.33
106	$C_3H_5Cl_3$	1,2,3-Trichloropropane	1.43241	0.38136	−0.02165	10	14843	42.87	56.04	66.32
107	C_3H_5I	3-Iodo-1-Propene	1.33639	0.24272	−0.02371	10	10000	35.96	53.70	72.21
108	C_3H_5N	Propionitrile	[redacted]			10	10000	3.46	8.77	18.68
109	C_3H_5NO	Hydracrylonitrile	1.50994	0.11037	—	10	105	41.72	53.79	—
110	C_3H_5NO	Lactonitrile	1.44156	0.32689	—	10	152	37.02	49.58	—
111	C_3H_6	Propylene	−0.93674	0.57775	−0.03853	10	10000	0.40	1.16	2.82
112	$C_3H_6Cl_2$	1,1-Dichloropropane	0.95379	0.28791	−0.02487	10	10000	16.48	26.92	39.24
113	$C_3H_6Cl_2$	1,2-Dichloropropane	0.98872	0.28700	−0.02571	10	10000	17.78	28.83	41.53
114	$C_3H_6Cl_2$	1,3-Dichloropropane	1.10340	0.27837	−0.02824	10	10000	22.57	35.25	48.35
115	$C_3H_6Cl_2$	2,2-Dichloropropane	0.85314	0.29432	−0.02255	10	10000	13.33	22.47	34.13
116	C_3H_6O	Acetone	[redacted]			10	10000	2.03	5.16	11.85
117	C_3H_6O	Allyl Alcohol	0.32390	0.49368	−0.04370	10	10000	5.94	13.69	25.80
118	C_3H_6O	n-Propionaldehyde	[redacted]			10	10000	3.23	7.53	14.37
119	C_3H_6O	1,2-Propylene Oxide	0.42829	0.53858	−0.02752	10	10000	1.21	3.46	8.20
120	C_3H_6O	1,3-Propylene Oxide	−0.50421	0.51872	−0.02296	10	10000	0.98	2.76	7.00
121	$C_3H_6O_2$	Ethyl Formate	0.12818	0.42260	−0.02090	10	10000	3.37	7.72	16.06
122	$C_3H_6O_2$	Methyl Acetate	0.13314	0.42849	−0.02188	10	10000	3.47	7.99	16.66
123	$C_3H_6O_3$	Propionic Acid	0.77846	0.44570	−0.05209	10	4872	14.86	28.94	44.34
124	$C_3H_6O_3S$	3-Mercaptopropionic Acid	1.68823	0.05916	—	10	66	55.90	—	—
125	$C_3H_6O_3$	Lactic Acid	1.60722	0.09225	—	10	107	50.06	61.90	—
126	$C_3H_6O_3$	Methoxyacetic Acid	1.61885	0.08873	—	10	71	51.00	—	—
127	C_3H_6S	Thiacyclobutane	0.67420	0.37225	−0.03151	10	10000	10.35	19.62	32.16
128	C_3H_7Br	1-Bromopropane	0.83601	0.32406	−0.02407	10	10000	13.68	24.43	39.04
129	C_3H_7Br	2-Bromopropane	0.81137	0.31043	−0.02155	10	10000	12.60	22.18	35.37
130	C_3H_7Cl	Isopropyl Chloride	0.31428	0.34779	−0.01661	10	10000	4.42	8.78	16.15
131	C_3H_7Cl	n-Propyl Chloride	0.40133	0.34678	−0.01833	10	10000	5.36	10.41	18.53
132	C_3H_7I	Isopropyl Iodide	1.26456	0.24157	−0.02122	10	10000	30.34	46.01	62.85
133	C_3H_7I	n-Propyl Iodide	1.30623	0.24227	−0.02250	10	10000	33.57	50.21	67.69
134	C_3H_7N	Allylamine	0.16250	0.39915	−0.02105	10	10000	3.46	7.49	14.71
135	C_3H_7N	Propyleneimine	0.06919	0.43329	−0.02293	10	10000	3.03	7.05	14.75
136	C_3H_7NO	N,N-Dimethylformamide	0.90253	0.37875	−0.04523	10	5220	17.22	30.14	42.83
137	$C_3H_7NO_2$	1-Nitropropane	0.91328	0.34648	−0.03730	10	10000	16.69	28.64	41.40
138	$C_3H_7NO_2$	2-Nitropropane	0.83248	0.35732	−0.03608	10	10000	14.25	25.28	37.99
139	C_3H_8	Propane	[redacted]			10	10000	0.47	1.23	2.89
140	C_3H_8O	Isopropanol	[redacted]			10	10000	5.00	11.30	21.53
141	C_3H_8O	n-Propanol	[redacted]			10	10000	6.63	14.69	26.42
142	$C_3H_8O_2$	2-Methoxyethanol	0.74339	0.41792	−0.04536	10	10000	13.06	24.99	38.81
143	$C_3H_8O_2$	Methylal	0.39079	0.38167	−0.01775	10	10000	3.59	7.64	15.00
144	$C_3H_8O_2$	1,2-Propylene Glycol	1.48275	0.11594	—	10	170	39.69	51.84	—
145	$C_3H_8O_2$	1,3-Propylene Glycol	1.38563	0.08395	—	10	58	46.73	—	—
146	C_3H_8S	n-Propylmercaptan	0.59031	0.31407	−0.02190	10	10000	7.63	13.52	21.65
147	C_3H_8S	Isopropyl Mercaptan	0.55779	0.31539	−0.02051	10	10000	7.12	12.78	20.86
148	C_3H_8S	Ethyl-Methyl-Sulfide	0.62830	0.31889	−0.02320	10	10000	8.39	14.90	23.78
149	C_3H_9N	n-Propylamine	0.05768	0.34918	−0.01241	10	10000	2.48	5.09	9.85
150	C_3H_9N	Isopropylamine	0.07464	0.37106	−0.01568	10	10000	2.69	5.68	11.14
151	C_3H_9N	Trimethylamine	[redacted]			10	10000	1.69	3.50	7.13
152	C_3H_9NO	1-Amino-2-Propanol	1.25496	0.27456	−0.04254	10	617	30.69	43.04	—
153	C_3H_9NO	3-Amino-1-Propanol	1.53733	0.08156	—	10	101	41.58	50.17	—
154	C_3H_9NO	Methylethanolamine	1.14745	0.30208	−0.04243	10	1422	25.53	38.18	46.97
155	$C_3H_9O_3P$	Trimethyl-Phosphite	1.00568	0.21001	−0.01402	10	10000	15.91	23.42	32.32
156	$C_3H_9O_4P$	Trimethyl Phosphate	1.48463	0.16933	−0.02290	10	1196	42.76	53.91	61.17
157	$C_3H_9N_2$	1,2-Propanediamine	0.90237	0.31904	−0.03400	10	10000	15.40	25.38	35.77
158	C_4H_4O	Furan	0.04084	[redacted]	[redacted]	10	10000	2.70	6.14	12.99
159	$C_4H_6O_2$	Diketene	0.87430	0.37094	−0.03962	10	10000	16.06	28.69	42.71
160	C_4H_4S	Thiophene	0.80753	0.32166	−0.02654	10	10000	12.67	22.12	34.17
161	C_4H_5Cl	Chloroprene	0.77957	0.29786	−0.02111	10	10000	10.15	17.41	27.11
162	C_4H_5N	trans-Crotonitrile	0.70791	0.37284	−0.03756	10	10000	11.05	20.11	30.79
163	C_4H_5N	cis-Crotonitrile	0.58131	0.39427	−0.03590	10	10000	8.70	16.84	27.61
164	C_4H_5N	Methacrylonitrile	0.46655	0.38890	−0.03042	10	10000	6.68	13.26	22.88
165	C_4H_5N	Pyrrole	0.83128	0.38413	−0.04217	10	10000	14.90	26.97	40.19
166	C_4H_5N	Vinylacetonitrile	0.61844	0.40844	−0.04032	10	10000	9.70	18.80	30.26
167	$C_4H_5NO_2$	Methyl Cyanoacetate	1.56587	0.09143	—	10	180	45.43	56.07	—
168	C_4H_6	1,3-Butadiene	−0.03359	0.34764	−0.01297	10	10000	2.00	4.07	7.81
169	C_4H_6	Dimethylacetylene	−0.06673	0.39387	−0.01524	10	10000	2.05	4.57	9.50
170	C_4H_6	Ethylacetylene	−0.02918	0.33636	−0.01056	10	10000	1.98	3.99	7.67
171	$C_4H_6Cl_2$	1,3-Dichloro-trans-2-Butene	1.30208	0.19939	−0.02091	10	10000	30.24	41.42	51.53
172	$C_4H_6Cl_2$	1,4-Dichloro-cis-2-Butene	1.40119	0.17876	−0.02041	10	5383	36.27	47.54	56.73

Table 1. Adsorption on Activated Carbon

No.	Formula	Name	Q = A + B Ln (ppm) + C (ppm)²			Q = g of compound/100 g of carbon ppmv in gas at 25 °C and 1 atm				
			A	B	C	Min	Max	Q @ 10 ppmv	Q @ 100 ppmv	Q @ 1000 ppmv
173	$C_4H_6Cl_2$	1,4-Dichloro-trans-2-Butene	1.40904	0.18120	−0.02179	10	4503	37.02	48.34	57.09
174	$C_4H_6Cl_2$	3,4-Dichloro-1-Butene	1.23394	0.21476	−0.02135	10	10000	26.75	37.85	48.54
175	C_4H_6O	trans-Crotonaldehyde	0.68353	0.36560	−0.03400	10	10000	10.35	19.00	29.81
176	[illegible]	2,5-Dihydrofuran	[illegible]	[illegible]	[illegible]	10	10000	5.20	11.03	20.92
177	C_4H_6O	Methacrolein	0.43461	0.32019	−0.02474	10	10000	6.03	11.91	21.01
178	$C_4H_6O_2$	gamma-Butyrolactone	[illegible]	[illegible]	[illegible]	10	592	35.07	50.39	—
179	$C_4H_6O_2$	cis-Crotonic Acid	1.30871	0.25008	−0.03752	10	773	33.21	45.58	—
180	$C_4H_6O_2$	Methacrylic Acid	1.23099	0.27648	−0.03903	10	1282	29.41	42.44	51.19
181	$C_4H_6O_2$	Methyl Acrylate	0.45869	0.32104	−0.02001	10	10000	5.75	10.49	17.45
182	$C_4H_6O_2$	Vinyl Acetate	0.61067	0.34797	−0.02595	10	10000	8.56	15.95	26.36
183	$C_4H_6O_3$	Acetic Anhydride	1.07388	0.33063	−0.03575	10	7274	22.33	35.69	48.37
184	[illegible]	n-Butyronitrile	[illegible]	[illegible]	[illegible]	10	10000	9.83	18.45	29.02
185	C_4H_7N	Isobutyronitrile	0.56697	0.38907	−0.03531	10	10000	8.31	15.92	25.90
186	C_4H_7NO	3-Methoxypropionitrile	1.13283	0.28534	−0.03732	10	2598	24.04	35.83	44.98
187	C_4H_8	1-Butene	0.07313	0.32701	−0.01412	10	10000	2.43	4.67	8.38
188	$C_4H_8Br_2$	1,2-Dibromobutane	1.69234	0.12766	−0.01437	10	4094	63.83	77.23	87.22
189	$C_4H_8Br_2$	2,3-Dibromobutane	1.68176	0.12916	−0.01412	10	4934	62.52	75.93	86.10
190	$C_4H_8Cl_2$	1,4-Dichlorobutane	1.38278	0.17795	−0.02010	10	5427	34.71	45.45	54.20
191	[illegible]	n-Butyraldehyde	[illegible]	[illegible]	[illegible]	10	10000	6.27	12.31	21.36
192	C_4H_8O	Isobutyraldehyde	0.39315	0.36715	−0.02379	10	10000	5.45	10.77	19.08
193	C_4H_8O	1,2-Epoxybutane	0.36719	0.37554	−0.02360	10	10000	5.25	10.61	19.25
194	[illegible]	Methyl Ethyl Ketone	[illegible]	[illegible]	[illegible]	10	10000	6.52	12.79	22.07
195	C_4H_8O	Ethyl Vinyl Ether	0.33311	0.39342	−0.01711	10	10000	4.47	8.59	15.25
196	[illegible]	Tetrahydrofuran	[illegible]	[illegible]	[illegible]	10	10000	14.36	8.90	16.03
197	$C_4H_8O_2$	Isobutyric Acid	1.14081	0.32004	−0.03833	10	2388	24.66	36.82	46.27
198	[illegible]	n-Butyric Acid	[illegible]	[illegible]	[illegible]	10	1244	28.40	40.37	48.30
199	$C_4H_8O_2$	1,4-Dioxane	[illegible]	[illegible]	−0.03034	10	10000	9.99	18.65	30.27
200	[illegible]	Ethyl Acetate	[illegible]	[illegible]	[illegible]	10	10000	8.99	16.49	26.74
201	$C_4H_8O_2$	Methyl Propionate	0.64273	0.34862	−0.02767	10	10000	9.20	16.96	27.52
202	$C_4H_8O_2$	n-Propyl Formate	0.65855	0.34340	−0.02750	10	10000	9.43	17.19	27.82
203	$C_4H_8O_2S$	Sulfolane	1.77762	0.00118	0.00005	10	10000	60.10	60.28	60.48
204	C_4H_8S	Tetrahydrothiophene	0.93777	0.33197	−0.03877	10	10000	17.02	27.97	38.44
205	C_4H_9Br	1-Bromobutane	1.16698	0.24380	−0.02270	10	10000	24.44	36.62	49.44
206	C_4H_9Br	2-Bromobutane	1.13872	0.24481	−0.02203	10	10000	22.99	34.69	47.30
207	C_4H_9Cl	n-Butyl Chloride	0.80024	0.29114	−0.02370	10	10000	11.69	19.40	28.87
208	C_4H_9Cl	sec-Butyl Chloride	0.75046	0.29132	−0.02212	10	10000	10.46	17.56	26.63
209	C_4H_9Cl	tert-Butyl Chloride	0.68873	0.28529	−0.01944	10	10000	8.97	15.12	23.92
210	[illegible]	Pyrrolidine	[illegible]	[illegible]	[illegible]	10	10000	8.73	16.37	26.76
211	C_4H_9NO	N,N-Dimethylacetamide	1.20076	0.35174	−0.03263	10	2631	26.23	37.34	45.74
212	C_4H_9NO	Morpholine	1.00473	0.30572	−0.03294	10	10000	19.03	30.65	42.41
213	[illegible]	n-Butane	[illegible]	[illegible]	[illegible]	10	10000	2.28	4.50	8.25
214	[illegible]	Isobutane	[illegible]	[illegible]	[illegible]	10	10000	2.02	4.00	7.47
215	$C_4H_{10}O$	n-Butanol	0.89881	0.32534	−0.03648	10	9276	15.41	25.33	35.20
216	[illegible]	sec-Butanol	[illegible]	[illegible]	[illegible]	10	10000	12.01	20.95	31.15
217	$C_4H_{10}O$	Diethyl Ether	0.23477	0.36044	−0.02236	10	10000	3.74	7.35	13.03
218	$C_4H_{10}O$	Methyl-Propyl-Ether	0.36764	0.32893	−0.01787	10	10000	4.77	9.00	15.62
219	$C_4H_{10}O$	Methyl Isopropyl Ether	0.36373	0.31940	−0.01647	10	10000	4.64	8.64	14.92
220	$C_4H_{10}O$	Isobutanol	0.84818	0.33355	−0.03559	10	10000	13.94	23.38	33.30
221	$C_4H_{10}O_2$	1,3-Butanediol	—	—	—	—	—	48.89	—	—
222	$C_4H_{10}O_2$	1,4-Butanediol	—	—	—	—	—	51.19	—	—
223	$C_4H_{10}O_2$	2,3-Butanediol	1.50442	0.09239	—	10	239	39.70	48.11	—
224	$C_4H_{10}O_2$	t-Butyl Hydroperoxide	1.08563	0.28496	−0.03035	10	7098	20.90	31.20	40.49
225	$C_4H_{10}O_2$	1,2-Dimethoxyethane	0.74981	0.31330	−0.02616	10	10000	10.89	18.70	28.46
226	$C_4H_{10}O_2$	2-Ethoxyethanol	1.07911	0.27792	−0.03119	10	6983	21.14	32.14	42.16
227	$C_4H_{10}O_4S$	Diethyl Sulfate	1.64797	0.03805	—	10	278	50.82	58.08	—
228	$C_4H_{10}S$	n-Butyl Mercaptan	0.98086	0.24388	−0.02211	10	10000	15.93	23.91	32.35
229	$C_4H_{10}S$	Isobutyl Mercaptan	0.93709	0.24802	−0.02179	10	10000	14.57	22.18	30.55
230	$C_4H_{10}S$	sec-Butyl Mercaptan	0.92287	0.24856	−0.02146	10	10000	14.12	21.59	29.88
231	$C_4H_{10}S$	tert-Butyl Mercaptan	0.84380	0.24937	−0.01939	10	10000	11.85	18.41	26.15
232	$C_4H_{10}S$	Diethyl Sulfide	0.95993	0.24465	−0.02193	10	10000	15.23	22.98	31.35
233	$C_4H_{10}S$	Isopropyl-Methyl-Sulfide	0.92769	0.24689	−0.02132	10	10000	14.23	21.69	29.95
234	$C_4H_{10}S$	Methyl-Propyl-Sulfide	0.97117	0.24453	−0.02229	10	10000	15.65	23.55	32.00
235	$C_4H_{10}S_2$	Diethyl Disulfide	1.42594	0.12564	−0.01373	10	5627	34.50	41.91	47.79
236	$C_4H_{11}N$	n-Butylamine	0.64570	0.31857	−0.02570	10	10000	8.68	15.14	23.45
237	$C_4H_{11}N$	Isobutylamine	0.60137	0.31538	−0.02369	10	10000	7.82	13.72	21.59
238	$C_4H_{11}N$	sec-Butylamine	0.57706	0.31254	−0.02250	10	10000	7.36	12.95	20.52
239	$C_4H_{11}N$	tert-Butylamine	0.50036	0.30334	−0.01897	10	10000	6.09	10.74	17.37
240	$C_4H_{11}N$	Diethylamine	0.54770	0.30799	−0.02107	10	10000	6.83	12.01	19.14
241	$C_4H_{11}NO$	Dimethylethanolamine	1.18381	0.23249	−0.02857	10	4183	24.42	34.24	42.09
242	$C_4H_{12}Si$	Tetramethylsilane	0.70867	0.23089	−0.01505	10	10000	8.40	12.89	18.45
243	$C_4H_{13}N_3$	Diethylene Triamine	1.54270	0.06479	—	10	308	40.50	47.02	—

stripper bed capacity is said to be 30 percent to 40 percent of equilibrium for plant operating conditions. The EPA Design Manual suggests a working factor of 3 for design of adsorption beds. The total carbon requirements for an adsorption system are obtained by determining carbon required from equilibrium capacity and then multiplying by the working factor.

Factors affecting adsorption bed capacity include loss due to adsorption zone, loss due to heat wave (adsorption is an exothermic process); loss due to moisture in entering gas and loss due to residual moisture on the carbon.

Carl L. Yaws is a professor of chemical engineering at Lamar University, Beaumont, Texas, and Li Bu and Sachin Nijhawan are graduate students at Lamar University. A computer program with data for all compounds is available for a fee from Yaws at 409-880-8787.

Reader Interest Review

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Appendix I

Air Emissions Basis for Additional Identified Hazardous Organic Constituents in the Hanford Tank Farms

CCN 128557

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R10593785

Memorandum

To: File - MS9-A

From: Edgardo Berríos

Ext: 371-3817

Fax:

Date: December 9, 2005

CCN: 128557

Subject: **AIR EMISSIONS BASIS FOR ADDITIONAL IDENTIFIED HAZARDOUS ORGANICS CONSTITUENTS IN THE HANFORD TANK FARMS**

References:
1) CHG 2004, *Industrial Hygiene Chemical Vapor Technical Basis*, RPP-22491, Rev 0, October 2004, CH2M HILL
2) 24590-WTP-M4C-FRP-00006, Rev B, *WTP Air Emissions Hazardous Organic Constituents Feed Concentrations*
3) 24590-WTP-RPT-PO-03-008, Rev 1, *Integrated Emissions Baseline Report for the Hanford Tank Waste Treatment and Immobilization Plant*
4) RPT-24590-EN00001, Rev 0, *Vessel Vents and PJM/RFD Emissions*
5) 24590-WTP-M4C-FRP-00005, *Estimation of Non-SSFM Represented Organic Emission Rates Required to Support the Integrated Emissions Baseline Report*
6) *Chemical Properties Handbook*, http://www.knovel.com
7) *Syracuse Research Corporation*, http://www.syrres.com/esc/physdemo.htm

Based on Reference 1, additional hazardous organic constituents, other than those already scoped through the WTP air permits, have been measured in Hanford tank headspaces. It is unknown if these constituents will be present in the WTP waste feed; therefore, the WTP and regulatory agencies have not determined if they will be included in the air permits and environmental risk evaluations. As the air emissions profile is currently being updated, it will be assumed for this update that these newly identified constituents are present in the WTP waste feed, and consequently their air emissions rates will be estimated. References 2 and 3 do not include the basis for these constituents; therefore, this memorandum serves as the documentation for these constituents basis.

The data (i.e. the basis) required to evaluate these constituents in the WTP air emissions flowsheet includes the following:

- Henry's Law constants - determines partition throughout the flowsheet and chemical group under which it is modeled.
- Appropriate modeling group per the guidelines established in References 3 and 4 - derived from the Henry's Law constants.

- Method detection limits - used to determine feed rate to the WTP.
- F_v values - used to determine unit operation removal efficiency throughout the WTP offgas systems (PT VV, PT PJV, LAW LOP/LVP, HLW HOP, and HLW PJV)

Per E&NS, the additional constituents to be evaluated are (from Reference 1, Tables 5-5 and 5-6):

CAS #	Organic Constituent
100-40-3	4-Ethenylcyclohexene
104-76-7	2-Ethyl-1-hexanol
10595-95-6	N-Nitrosomethylethylamine
109-74-0	Butanenitrile
110-59-8	Pentanenitrile
123-72-8	Butanal
134-32-7	alpha-Napthylamine
589-38-8	3-Hexanone
628-73-9	Hexanenitrile
75-02-5	Fluoroethene
79-46-9	2-Nitropropane

The basis for each constituent was established as follows:

Henry's Law constants

An Internet search was made to obtain the Henry's Law constant. The site used was the Syracuse Research Corporation website (Ref. 7). Results from each organic constituent search are provided in Attachment A and summarized below.

CAS#	Organic Constituent	Henry's Law Constant (atm-m^3/mole)
100-40-3	4-Ethenylcyclohexene	4.48E-02
104-76-7	2-Ethyl-1-hexanol	2.65E-05
10595-95-6	N-Nitrosomethylethylamine	1.44E-06
109-74-0	Butanenitrile	5.23E-05
110-59-8	Pentanenitrile	7.15E-05
123-72-8	Butanal	1.15E-04
134-32-7	alpha-Napthylamine	1.11E-07
589-38-8	3-Hexanone	1.25E-04
628-73-9	Hexanenitrile	9.49E-05
75-02-5	Fluoroethene	1.18E-01
79-46-9	2-Nitropropane	1.19E-04

Modeling Group

Per Reference 4, all organic constituents were organized into groups of similar physical properties. Representative compounds from each group were selected and modeled in the air

emissions flowsheet. This was done to avoid complexity of the flowsheet. Based on the results from the modeled constituents, the air emission rates for the non-modeled constituents are then calculated as they are assumed to behave similarly during vapor-liquid equilibrium conditions. Therefore, these new constituents need to be included into their pertaining group. The main criterion for the grouping was similar Henry's Law constants. Based on this methodology, the new identified hazardous organic constituents fall within the following groups:

CAS#	Organic Constituent	Group
100-40-3	4-Ethenylcyclohexene	22
104-76-7	2-Ethyl-1-hexanol	12
10595-95-6	N-Nitrosomethylethylamine	9
109-74-0	Butanenitrile	13
110-59-8	Pentanenitrile	13
123-72-8	Butanal	15
134-32-7	alpha-Napthylamine	6
589-38-8	3-Hexanone	15
628-73-9	Hexanenitrile	14
75-02-5	Fluoroethene	23
79-46-9	2-Nitropropane	15

Method Detection Limit

Detection limits are used to determine the concentration of the constituent in the waste feed as documented in Reference 2. No detection limits are readily available for these constituents therefore the approach taken is to assume that the constituents method detection limit will be the same to the method detection limit from a comparable compound found in the feed stream. For example, for 3-Hexanone, the method detection limit is assumed to be the same as for 3-Heptanone and for 2-Nitropropane, the method detection limit is assumed to be the same as for 1-Nitropropane. For the nitriles, the method detection limit was assumed to be the highest of all the nitriles in the feed which turned out to be acrylonitrile. After evaluating the new constituents against the existing constituents, the following detection limits were selected:

CAS#	Organic Constituent	Method Detection Limit (mg/L)	Constituent Used As Basis for Method Detection Limit
100-40-3	4-Ethenylcyclohexene	0.02	Cyclohexene
104-76-7	2-Ethyl-1-hexanol	0.07	Ethyl alcohol
10595-95-6	N-Nitrosomethylethylamine	0.3	N-Nitroso-di-n-propylamine
109-74-0	Butanenitrile	0.1	Acrylonitrile
110-59-8	Pentanenitrile	0.1	Acrylonitrile
123-72-8	Butanal	0.066	1,2-Epoxybutane
134-32-7	alpha-Napthylamine	0.066	Triethylamine
589-38-8	3-Hexanone	0.02	3-Heptanone
628-73-9	Hexanenitrile	0.1	Acrylonitrile
75-02-5	Fluoroethene	0.066	Chloropentafluoroethane
79-46-9	2-Nitropropane	0.3	1-Nitropropane

Per Table 4 of Reference 2, the adjusted concentrations of these constituents to arrive at the assumed total organic carbon weight percent in the feed are:

CAS#	Organic Constituent	Adjusted Feed Concentration (mg/L)
100-40-3	4-Ethenylcyclohexene	4
104-76-7	2-Ethyl-1-hexanol	10
10595-95-6	N-Nitrosomethylethylamine	60
109-74-0	Butanenitrile	20
110-59-8	Pentanenitrile	20
123-72-8	Butanal	10
134-32-7	alpha-Napthylamine	10
589-38-8	3-Hexanone	4
628-73-9	Hexanenitrile	20
75-02-5	Fluoroethene	10
79-46-9	2-Nitropropane	60

F_v values

F_v is a unitless parameter used to classify a constituent as being in one of three categories: vapor phase, particle phase, or particle-bound phase. This phase type affects the removal efficiency of the offgas control system for that compound. An F_v value of 1 indicates that the constituent exists only in the vapor phase. If the F_v value is less than 1, for example 0.9, this means that 90% of the compound exits in the vapor phase and 10% is particle-bound (i.e. [1-0.9]*100%). Therefore, removal efficiency for each portion of the constituent will differ based on the phase. Based on E&NS evaluations of each constituent's vapor pressure and melting point, the F_v values have been calculated to be 1 for all the constituents.

The decontamination factors (DFs) for these constituents for each unit operation will be the same as those for other vapor constituents in all unit operations except for the Pretreatment thermal oxidizer and carbon beds, which are calculated based on the constituent's properties. The DFs for these constituents are:

LAW

- Melter: 1.1
- SBS: 1
- WESP: 1
- HEPA: 1
- Carbon Beds: 1
- SCO: 20
- SCR: 1
- Caustic Scrubber: 1

HLW

- Melter: 1.1
- SBS: 1
- WESP: 1
- HEME: 1
- HEPA: 1
- Carbon Beds: 1
- Silver Mordenite: 1
- SCO: 20
- SCR: 1
- PJV HEPA: 1

Pretreatment

- Caustic Scrubber: 1
- HEME: 1
- HEPA: 1
- Thermal Oxidizer: calculated below
- Carbon Bed: calculated below
- PJV Demister: 1
- PJV HEPA: 1

The DFs for the Pretreatment thermal oxidizer and carbon beds depend on the auto ignition temperatures (AIT), boiling points, and molecular weights of each constituent. The methodology of calculating these DFs is explained in Appendix G of Reference 3. The AITs were obtained from the Chemicals Property Handbook located in Reference 6. When no data was available for a constituent, the AIT for the constituent used to obtain the method detection limit was used. When this situation occurred, the AITs were obtained from Table 1-1 in Appendix G of Reference 3.

The removal efficiency of the thermal oxidizer is based on the temperature difference between the operating temperature of the thermal oxidizer and the AIT of the constituent. Therefore, the higher the difference between the temperatures, the more efficient the unit is in destroying the organic constituent. The operating temperature of the thermal oxidizer is 1600°F. The AITs and the difference between that temperature and the operating temperature of the thermal oxidizer are:

CAS#	Organic Constituent	AIT (°F)	°F Difference from TO Operating Temperature
100-40-3	4-Ethenylcyclohexene	518	1082
104-76-7	2-Ethyl-1-hexanol	550	1050
10595-95-6	N-Nitrosomethylethylamine	527	1073
109-74-0	Butanenitrile	935	665
110-59-8	Pentanenitrile	897.8	702.2
123-72-8	Butanal	446	1154

CAS#	Organic Constituent	AIT (°F)	°F Difference from TO Operating Temperature
134-32-7	alpha-Napthylamine	**480**	1120
589-38-8	3-Hexanone	**734**	866
628-73-9	Hexanenitrile	**897.8**	702.2
75-02-5	Fluoroethene	725	875
79-46-9	2-Nitropropane	802	798

The AITs in bold indicate that these AITs are from the constituents used to determine the method detection limit.

Per the guidelines in Appendix G of Reference 3, for temperature differences between the AIT and thermal oxidizer operating range over 650°F, the expected thermal oxidizer removal efficiency is 99.99% (i.e. DF = 10,000). This indicates that all the constituents will have a DF of 10,000 in the Pretreatment thermal oxidizer.

For the carbon beds, the removal efficiency depends on the loading in the carbon beds, which is dependent on the organic constituent boiling point and molecular weight. Based on these values, the guidelines presented on Tables G-3 and G-4 of Appendix G in Reference 3 were applied to determine the removal efficiency for the constituent. The results are as follows:

CAS#	Boling Point (°C)	Molecular Weight (g/mole)	Adsorption Capability (g/100g carbon)	Carbon Bed Removal Efficiency (%)	Carbon Bed DF
100-40-3	128	108.18	2	80	5
104-76-7	184.6	130.23	10	95	20
10595-95-6	170	88.11	20	98	50
109-74-0	117.6	69.11	2	80	5
110-59-8	141.3	83.13	2	80	5
123-72-8	74.8	72.11	1	50	2
134-32-7	300.8	143.19	40	98	50
589-38-8	123.5	100.16	10	95	20
628-73-9	163.6	97.16	10	95	20
75-02-5	-72	46.05	0	0	1
79-46-9	120.2	89.1	2	80	5

Boiling points and molecular weights were obtained from Attachment 1 of this memorandum.

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If these constituents are required to be included in the waste feed in the future, the bases presented in this memorandum will be included in References 2, 3, and 5.

Edgardo Berríos
Process Engineer
Process Engineering - Flowsheet and ORP Deliverables

EB/eb

Attachment: Organic Constituents Physical Properties Data

Distribution

Copy Coverage	MSIN
Berríos, E	MS4-C1
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Saunders, S	MS4-C1

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value. References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000100-40-3
Chem Name  : 4-VINYLCYCLOHEXENE
Mol Formula: C8H12
Mol Weight : 108.18
Melting Pt : -108.9 deg C
Boiling Pt : 128 deg C
Water Solubility:
   Value : 50 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 3.93
   Type  : EXP
   Ref   : CHEM INSPECT TEST INST (1992)
Vapor Pressure:
   Value : 15.7 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.0448 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 8.93E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000104-76-7
Chem Name  : 2-ETHYL-1-HEXANOL
Mol Formula: C8H18O
Mol Weight : 130.23
Melting Pt : -70 deg C
Boiling Pt : 184.6 deg C
Water Solubility:
   Value : 880 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : AMIDON,GL ET AL. (1974)
Log P (octanol-water):
   Value : 2.73
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 0.136 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 2.65E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 1.32E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 010595-95-6
Chem Name  : N-METHYL-N-NITROSOETHAMINE
Mol Formula: C3H8N2O
Mol Weight : 88.11
Melting Pt :
Boiling Pt : 170 deg C
Water Solubility:
   Value : 3E+005 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : IARC (1978)
Log P (octanol-water):
   Value : 0.04
   Type  : EXP
   Ref   : VERA,A ET AL. (1992)
Vapor Pressure:
   Value : 1.1 mm Hg
   Temp  : 20 deg C
   Type  : EST
   Ref   : KLEIN,RG (1982)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 1.44E-006 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : ATKINSON,R (1988)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000109-74-0
Chem Name  : BUTYRONITRILE
Mol Formula: C4H7N
Mol Weight : 69.11
Melting Pt : -111.9 deg C
Boiling Pt : 117.6 deg C
Water Solubility:
   Value : 3.3E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : RIDDICK,JA ET AL. (1986)
Log P (octanol-water):
   Value : 0.53
   Type  : EXP
   Ref   : TANII,H & HASHIMOTO,K (1984)
Vapor Pressure:
   Value : 19.5 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 5.23E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BUTLER,JAV AND RAMCHANDANI,CN (1935)
Atmospheric OH Rate Constant:
   Value : 7.56E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : ATKINSON,R (1988)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value. References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000110-59-8
Chem Name  : VALERONITRILE
Mol Formula: C5H9N
Mol Weight : 83.13
Melting Pt : -96.2 deg C
Boiling Pt : 141.3 deg C
Water Solubility:
   Value : 7750 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 1.12
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 7.3 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 7.15E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 1.67E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

Abbreviations in the 'Type' field: EXP = Experimental Data, EST = Estimated Data, EXT = Extrapolated Data. Extrapolated data is based upon experimental measurement outside the temperature range of the reported value. References below are abbreviated citations ... the full reference citations are NOT available here. References for Estimated data generally refer to the method used to make the estimate ... most estimates were made using SRC software.

```
CAS Number : 000123-72-8
Chem Name  : BUTYRALDEHYDE
Mol Formula: C4H8O
Mol Weight : 72.11
Melting Pt : -99 deg C
Boiling Pt : 74.8 deg C
Water Solubility:
   Value : 7.1E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : UNION CARBIDE (1974)
Log P (octanol-water):
   Value : 0.88
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 111 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1985)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000115 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BUTTERY,RG ET AL. (1969)
Atmospheric OH Rate Constant:
   Value : 2.35E-011 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1985)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000134-32-7
Chem Name  : 1-NAPHTHYLAMINE
Mol Formula: C10H9N
Mol Weight : 143.19
Melting Pt : 49.2 deg C
Boiling Pt : 300.8 deg C
Water Solubility:
   Value : 1700 mg/L
   Temp  : 20 deg C
   Type  : EXP
   Ref   : DRAGUN,J & HELLING,CS (1985)
Log P (octanol-water):
   Value : 2.25
   Type  : EXP
   Ref   : HANSCH,C ET AL. (1995)
Vapor Pressure:
   Value : 0.00418 mm Hg
   Temp  : 25 deg C
   Type  : EXT
   Ref   : CHAO,J ET AL. (1983)
pKa Dissociation Constant:
   Value : 3.92
   Temp  : 25 deg C
   Type  : EXP
   Ref   : WEAST,RC (1985)
Henry's Law Constant:
   Value : 1.11E-007 atm-m3/mole
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ABRAHAM,MH ET AL. (1994)
Atmospheric OH Rate Constant:
   Value : 2E-010 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000589-38-8
Chem Name  : 3-HEXANONE
Mol Formula: C6H12O
Mol Weight : 100.16
Melting Pt : -55.5 deg C
Boiling Pt : 123.5 deg C
Water Solubility:
   Value : 1.47E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Log P (octanol-water):
   Value : 1.24
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 13.9 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : YAWS,CL (1994A)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.000125 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 6.9E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000628-73-9
Chem Name  : HEXANENITRILE
Mol Formula: C6H11N
Mol Weight : 97.16
Melting Pt : -80.3 deg C
Boiling Pt : 163.6 deg C
Water Solubility:
   Value : 2480 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 1.66
   Type  : EXP
   Ref   : TANII,H & HASHIMOTO,K (1984)
Vapor Pressure:
   Value : 2.85 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 9.49E-005 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 3.09E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1993)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000075-02-5
Chem Name  : VINYLFLUORIDE
Mol Formula: C2H3F
Mol Weight : 46.05
Melting Pt : -160.5 deg C
Boiling Pt : -72 deg C
Water Solubility:
   Value : 1.29E+004 mg/L
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM ET AL. (1996)
Log P (octanol-water):
   Value : 1.19
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1995)
Vapor Pressure:
   Value : 1.98E+004 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1989)
pKa Dissociation Constant:
   Value :
   Temp  :
   Type  :
   Ref   :
Henry's Law Constant:
   Value : 0.118 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : MEYLAN,WM & HOWARD,PH (1991)
Atmospheric OH Rate Constant:
   Value : 5.56E-012 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : ATKINSON,R (1989)
```

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Data From SRC PhysProp Database:

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```
CAS Number : 000079-46-9
Chem Name  : 2-NITROPROPANE
Mol Formula: C3H7NO2
Mol Weight : 89.10
Melting Pt : -91.3 deg C
Boiling Pt : 120.2 deg C
Water Solubility:
   Value : 1.7E+004 mg/L
   Temp  : 25 deg C
   Type  : EXP
   Ref   : BAKER,PJJR & BOLLMEIER,AFJR (1981)
Log P (octanol-water):
   Value : 0.93
   Type  : EXP
   Ref   : CHEM INSPECT TEST INST (1992)
Vapor Pressure:
   Value : 17.2 mm Hg
   Temp  : 25 deg C
   Type  : EXP
   Ref   : DAUBERT,TE & DANNER,RP (1987)
pKa Dissociation Constant:
   Value : 7.68
   Temp  : 25 deg C
   Type  : EXP
   Ref   : SERJEANT,EP & DEMPSEY,B (1979)
Henry's Law Constant:
   Value : 0.000119 atm-m3/mole
   Temp  : 25 deg C
   Type  : EST
   Ref   : VP/WSOL
Atmospheric OH Rate Constant:
   Value : 2.6E-013 cm3/molecule-sec
   Temp  : 25 deg C
   Type  : EXP
   Ref   : LIU,R ET AL. (1990)
```

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ISSUED BY
RPP-WTP PDC
INIT 7/16/03
DATE

Calculation Cover Sheet

RIVER PROTECTION PROJECT-WASTE TREATMENT PLANT			JOB NO.: 24590		
CALC NO. 24590-WTP-HAC-50-00001			GROUP E&NS		
SUBJECT Estimated Organic Emissions from Process Cells					
CALCULATION STATUS DESIGNATION	☒ PRELIMINARY ☐ SUPERSEDED	☐ COMMITTED PRELIMINARY		☐ CONFIRMED ☐ VOIDED	
COMPUTER PROGRAM/TYPE	N/A ☒	SCP ☐ YES ☐ NO	☐ STAND-ALONE ☐ NETWORKED	PROGRAM NAME	VERSION/RELEASE NO.

Notes/Comments

The software tool used was Microsoft Excel Version 97.

Originator – John Sipkowski
Reviewer – Lee Bostic
Approver – Phil Peistrup

NO.	REASON FOR REVISION	TOTAL NO OF SHEETS	LAST SHEET NO	BY	CHECKED	APPROVED/ ACCEPTED	DATE
C	Preliminary Calculation. Complete revision based upon updated source data. Reformatted to include Excel tables as an appendix.	39	A-29	J. Sipkowski	L. Bostic	P. Peistrup	7/14/03
B	Preliminary Calculation. Table 1 from Version A deleted. The summary was revised accordingly.	47	47	J. Sipkowski	L. Bostic	P. Peistrup	10/3/02 7-15-03
A	Preliminary Calculation	48	48	J. Sipkowski	L. Bostic	P. Peistrup	8/22/02 7-15-03

RECORD OF REVISIONS

Please note that source, special nuclear, and byproduct materials, as defined in the Atomic Energy Act of 1954 (AEA) are regulated at the U. S. Department of Energy (DOE) facilities exclusively by DOE acting pursuant to its AEA authority. DOE asserts that pursuant to AEA, it has sole and exclusive responsibility and authority to regulate source, special nuclear, and byproduct materials at DOE-owned nuclear facilities. Information contained herein on radionuclides is provided for process description purposes only.

CALCULATION SHEET

PROJECT: RPP-WTP
JOB NO.: 24590
CALC NO.: 24590-WTP-HAC-50-00001
SHEET REV: C
SHEET NO.: 1

BY: John Sipkowski
DATE: July 9, 2003

SUBJECT: Estimated Organic Emissions from Process Cells

Contents

Sheet 1. Contents and Acronyms

Sheet 2. Discussion

Sheet 8. References

Sheet 10. Appendix A. Excel Worksheets: Table 1 through Table 9

Acronyms

EPA	US Environmental Protection Agency
HEPA	high efficiency particulate air (filter)
HLW	high-level waste
LAW	low-activity waste
PICs	products of incomplete combustion
SOCMI	synthetic organic chemical manufacturing industry
WAC	Washington Administrative Code
WTP	Hanford Tank Waste Treatment and Immobilization Plant

BY: John Sipkowski
DATE: July 9, 2003

SUBJECT: Estimated Organic Emissions from Process Cells

Summary

This calculation estimates the potential emission of organic compounds from ancillary equipment located within the Hanford Tank Treatment and Immobilization Plant (WTP) process cells. First, the release of organic compounds from ancillary equipment into the process cells was estimated. The release amount was then apportioned to each individual organic compound. Only a portion of the released organic material will result in uncontrolled emission. Particulate and particle-bound organics will be abated by the HEPA filters in the process cell offgas treatment system. The vapor phase will not be abated by the HEPA filters and will comprise the potential organic emissions from the process cells.

1 Introduction

This calculation estimates the potential emission of organic compounds from the WTP process cells as a result of treating the Hanford tank waste. The process cells will be operated under negative pressure with respect to atmospheric pressure, and the air from the process cells will be released to the atmosphere through a stack or flue. According to the Washington Administrative Code (WAC), WAC 173-400-030(32), fugitive emissions "means emissions which do not pass and which could not reasonably pass through a stack, chimney, vent, or other functionally equivalent opening." Consequently, the Washington State Department of Ecology (Ecology) has agreed (CCN 023430) that fugitive emissions are not applicable to the WTP. However, Ecology requested that the WTP estimate the potential emission of organic compounds that are not abated by the WTP offgas treatment systems.

In response to that request, this calculation estimates the potential unabated emission of organic compounds from the WTP process cells. This estimate is based upon Environmental Protection Agency (EPA) guidance documents. The emission estimate was made using the following process:

- Estimate the annual release of organic material into the process cells from ancillary equipment for the pretreatment plant, the low-activity waste (LAW) vitrification plant, and the high-level waste (HLW) vitrification plant
- Determine the weight fraction of individual organic compounds in the streams being evaluated
- Apportion the annual release of organic material to the individual organic compounds
- Apply ventilation abatement to the applicable organic compounds

This process resulted in an estimate of the potential emission of each organic compound from the pretreatment plant, the LAW plant, and the HLW plant process cells given in Appendix A, Tables 7, 8, and 9, respectively.

The scope of this calculation is limited to providing an estimate of potential organic compound emission from process cells to support the WTP risk assessment process.

2 Release Calculation Methodology

Building ventilation and process offgases will be treated by abatement systems that employ best available control technology for criteria pollutants, radionuclides, and toxic air pollutants prior to discharge into the atmosphere through a stack or flue. Organic compounds may be released into the process cells from ancillary equipment. Process cell ventilation will be treated by high efficiency particulate air (HEPA)

filters that will abate particulate or particle bound organic compounds. Vapor phase organic compounds will not be abated by the HEPA filters and are considered in this calculation to be process cell organic emissions.

The following sections present the formula for estimating the release of organic compounds from ancillary equipment within process cells and describes adjustments to the formula based upon the design and operation of the WTP.

2.1 Release Calculation Formula

The estimated release of organic material from ancillary equipment was calculated using the EPA guidance document, *Protocol for Equipment Leak Emission Estimates* (EPA 1995). This guidance provides several different methods to determine releases. The guidance recommends using the method that best matches the type of process being evaluated and the data available on that process. Since the WTP is not in operation, actual release measurements are not available, thus average release factors, given in the guidance, were used for the calculation. The formula for estimating releases using the average release factors is:

$$E_{HO} = N \cdot R_{avg} \cdot WF_s \cdot H$$

Where:

E_{HO} = estimated annual release of organic compounds, kg/year
N = ancillary equipment count by equipment type
R_{avg} = average release factor by equipment type, kg/hour
H = hours of operation, hours/year
WF_S = weight fraction of organic material by waste stream

An explanation of each formula value is discussed in the following sections, and the calculations are presented in Appendix A, Table 1.

2.2 Count of Ancillary Equipment by Equipment Type

The EPA guidance (EPA 1995) determined that the following ancillary equipment types are sources of potential release:

- Valves
- Pump seals
- Compressor seals
- Pressure relief valves
- Connectors
- Agitator seals
- Open-ended lines
- Sampling connections

The potential to emit for each of these ancillary equipment types are discussed below as they pertain to the design and operation of the WTP.

Valves

Valves that contact the waste were included in the release estimate.

Pumps

Reverse flow diverter pumps were not considered in this calculation since these offgases will be captured in process vessel ductwork, treated by the offgas treatment train, and released from the plant stack. The resultant estimated emissions are already included in the *Integrated Emissions Baseline Report for the Hanford Tank Waste Treatment and Immobilization Plant (*Emission Baseline Report) (24590-WTP-RPT-PO-03-008).

The WTP will also use conventional, centrifugal pumps. Centrifugal pumps that contact the waste will be equipped with double mechanical seals with an inert barrier fluid at greater pressure than the waste. It is assumed that there is no potential for releases from these pumps.

Compressors

The design of the WTP does not include compressors that contact the waste.

Pressure relief valves

Pressure relief valves on the process vessels and tanks were not considered sources of release in this calculation since all of the process vessels and tanks that manage the Hanford tank waste will operate under one to two inches of water gauge vacuum. The EPA guidance (EPA 1995) considers equipment under vacuum to be zero release.

Connections

Welded connections are considered to be zero release in the EPA guidance (EPA 1995). Other types of connectors such as gasketed flanged connections that contact the waste were included in this release estimate.

Agitator seals

Most of the process vessels that are agitated will use pulse jet mixers located within the vessels being agitated. Emissions from pulse jet mixers were not considered in this calculation since these offgases will be captured in the process vessel ductwork, treated by the offgas treatment train, and released from the plant stacks. The resultant estimated emissions are already included in the Emission Baseline Report (24590-WTP-RPT-PO-03-008).

Certain vessels will employ mechanical agitators that do employ a seal. These seals will be in the vapor space of the vessel, and the vessels will be under one to two inches of water gauge vacuum. The EPA guidance (EPA 1995) considers equipment under vacuum to be zero release.

Open-ended lines

The design of the WTP does not include open-ended lines.

Sampling systems

Sampling systems in the WTP will be closed-loop and are considered in the EPA guidance (EPA 1995) to be zero emission.

Thus, this calculation includes release calculations for valves and gasketed flanged type connectors that will contact the Hanford tank waste.

The ancillary equipment count by equipment type, N, is given in Appendix A, Table 1. The count of connectors that contact the Hanford tank waste was provided by Melter Systems (CCN 068046, CCN 068047) and the Pretreatment Jumper Group (CCN 068045). The count of valves was taken from the Plant Item List (PIL-4.08.06).

2.3 Average Release Factors

The EPA developed the average release factors through extensive measurements of actual processes in operation. This calculation used average release factors developed for the synthetic organic chemical manufacturing industry (SOCMI) since the processes proposed for the WTP are similar to the processes used in SOCMI.

The SOCMI average release factors for valves are based upon the type of service. The EPA guidance (EPA 1995) defines the types of service as:

- Gas/vapor – material in a gaseous state at operating conditions;
- Light liquid – material in a liquid state in which the sum of the concentrations of individual constituents with a vapor pressure over 0.3 kilopascals at 20° C is greater than or equal to twenty weight percent; or,
- Heavy liquid – not in gas/vapor service or light liquid service.

The release factor for heavy liquid service was used in this calculation since the *RPP-WTP Waste Feed Assessment* report (RPT-24590-EN00003) determined the total organic carbon content of the Hanford waste to be bounded at four weight percent.

The average release factor for connectors is the same regardless of the type of service. The average release factors, R_{avg}, applicable to the WTP are shown in Appendix A, Table 1.

2.4 Weight Fraction of Organic Material

The EPA guidance (EPA 1995) states that the weight fraction must be determined for each waste stream under evaluation. Four waste streams were evaluated for the calculation of ancillary equipment releases. These four waste streams are:

(1) The waste feed from receipt through the pretreatment evaporator process labeled the "pretreatment feed stream"
(2) The waste stream after the pretreatment evaporator labeled the "post-evaporator stream"
(3) The LAW concentrate through the LAW vitrification process labeled the "LAW stream"
(4) The HLW concentrate through the HLW vitrification process labeled the "HLW stream"

Section 3 addresses the determination of the weight fraction of the individual organic compounds in each of the four evaluated streams. The individual weight fractions were summed for each of the evaluated streams and entered onto Appendix A, Table 1 as the respective waste stream organic weight fraction, WF_S.

2.5 Hours of Operation

The calculation will use 8760 hours of operation which represents continuous operation for a year. The operating hours used is conservative since the average operational availability of the WTP is approximately 71% as determined in *LAW Vitrification Capacity and Availability Study* (24590-LAW-RPT-ENG-01-001). In addition, most of the transfer pipes will remain empty between transfers and will be flushed with water after transfer to prevent solids from settling in the line and to minimize corrosion.

2.6 Estimated Release of Organic Material

Appendix A, Table 1 gives the estimated release of organic material, E_{HO}, into the process cells of the pretreatment plant feed and post-evaporator streams, the LAW stream, and the HLW stream as a result of applying the average release calculation formula.

3 Weight Fraction of Individual Organic Compounds

The following sections discuss the determination of the weight fraction of each organic compound in each of the four evaluated streams.

3.1 Weight Fraction of Organic Compounds in the Pretreatment Feed Stream

The *RPP-WTP Waste Feed Assessment* (RPT-24590-EN00003) determined the upper bound concentration of individual organic compounds in the Hanford waste feed to the WTP. These concentrations are the starting point for the organic emissions calculations from the three production plants. The concentrations were given in milligrams per liter, mg/L. The formula given in the EPA guidance (1995) in section 2.1 to estimate the release of organic compounds requires the organic concentration to be expressed as a weight fraction. The milligrams per liter, mg/L, were converted to weight fractions, mg/kg, using the density, ρ, of the waste provided in the *RPP-WTP Waste Feed Assessment* (RPT-24590-EN00003). The values are given in Appendix A, Table 2. The individual weight fractions were summed in Appendix A, Table 2 to yield the waste stream organic weight fraction, WF_S, for the pretreatment feed stream and entered onto Appendix A, Table 1.

3.2 Weight Fraction of Organic Compounds in the Post-Evaporator, LAW, and HLW Streams

The Emission Baseline Report (24590-WTP-RPT-03-008) estimated the mass flow rate of fifty organic compounds in the waste using a computer model. The fifty organic compounds were selected as representative of the full spectrum of organic compounds in the waste. These fifty organic compounds were organized into thirty-five groups, termed Henry's Grouping, based upon the similarity of properties such as Henry's Law constant, molecular weight, vapor pressure, and solubility. The unmodeled organic compounds in the waste were assigned to one of the thirty-five groups based upon that compound's similar Henry's Grouping properties.

The model estimated the mass flow rate for each of the fifty organic compounds in the post-evaporator, the LAW, and the HLW streams shown in Appendix A, Tables 2, 3, and 4, respectively. Each unmodeled organic compound was then assigned, by stream, a mass flow rate associated with the appropriate Henry's Grouping. Some of the Henry's Groupings contain more than one modeled compound. In that case, the mass flow rates were averaged, and the average value was assigned to the unmodeled organic compounds in that Henry's Grouping. Appendix A, Table 6 shows the Henry's Grouping number and corresponding mass flow rate assigned to each organic compound, both modeled and unmodeled, in the post-evaporator stream; Appendix A, Table 8 shows the LAW stream; and Appendix A, Table 9 shows the HLW stream.

The formula given in the EPA guidance (1995) in section 2.1 to estimate the release of organic compounds requires the organic concentration to be expressed as a weight fraction. The mass flow rates were converted to weight fractions using the respective density for the three streams. The density used for this calculation is the density of the liquid phase of the waste stream being evaluated since the model apportioned the organic compounds to the liquid phase. A conversion factor was calculated to convert from mass flow rate to weight fraction according to the following formula:

$$\text{Conversion Factor} = Q_M \text{ g/s} \cdot 60 \text{ s/min} \cdot \text{min}/Q_V \cdot 35.315 \text{ ft}^3/1000\text{L} \cdot 1000 \text{ mg/g} \cdot 1/\rho \text{ kg/L}$$

Where:
Q_M = mass flow rate of the individual organic compound
Q_V = volumetric flow rate of the evaluated stream
ρ = density of the liquid phase of the evaluated stream

Appendix A, Table 6 shows the mass flow rate and conversion to a weight fraction for each of the organic compounds for the post-evaporator stream. The individual weight fractions were summed to yield the waste stream organic weight fraction, WF_S, for the post-evaporator stream. Appendix A, Table 8 presents the same information for the LAW stream, and Appendix A, Table 9 presents the same information for the HLW stream. The waste stream organic weight fractions, WF_S, for each of the evaluated streams was entered into Appendix A, Table 1.

4 Estimated Release of Organic Compounds

The *Human Health Risk Assessment Protocol* (EPA 1998) presents a method to speciate the release of organic compounds by multiplying the weight ratio of each individual organic compound by the total release from the waste streams being evaluated. This method was used to estimate the individual organic compound released into the WTP process cells for each of the evaluated streams.

The weight ratio for each organic compound for each stream was determined by dividing the individual organic compound weight fraction by the total weight fraction of all organic compounds in that stream.

The estimated release of each individual organic compound for each stream, R_{IO}, was then determined by multiplying the estimated release for the stream, ER_O, from Appendix A, Table 1 times the individual organic compound weight ratio, WR_i. These calculations were made for the pretreatment feed stream, the post-evaporator stream, the LAW stream, and the HLW stream. The resulting estimated releases into the process cells are given in Appendix A, Tables 5, 6, 8, and 9, respectively.

5 Estimated Emission of Organic Compounds

This section discusses the calculation of the estimated emission of organic compounds from the WTP process cells.

5.1 Unabated Organic Compound Emissions

Only a portion of the organic compound released into the process cells will result in unabated emissions. Organic compounds that are particle-bound or particulate will be abated by the high-efficiency particulate air (HEPA) filters. The Emission Baseline Report (24590-WTP-RPT-03-008) separated the organic compounds into particle-bound or particulate, and vapor phase. According to the Emission Baseline Report (24590-WTP-RPT-03-008), HEPA filters will abate the particle-bound or particulate organic compounds at a decontamination factor of two hundred thousand. Therefore, particle-bound or particulate organic compounds were not considered as uncontrolled emissions in this calculation.

Vapor phase organic compounds released into the process cells will not be captured by the HEPA filters and will represent potential unabated emissions. Appendix A, Table 5 gives the estimated organic vapor emission, R_{VO}, from the pretreatment feed stream by listing the release of each vapor phase organic compound as an emission and each particle-bound or particulate organic compound as zero emission. This process is repeated for the post-evaporator stream in Appendix A, Table 6. The feed stream and post-evaporator stream releases are summed in Appendix A, Table 7 to give the estimated emission of organic compounds from the pretreatment process cells. Appendix A, Table 8 gives the estimated emission of organic compounds from the LAW process cells, and Appendix A, Table 9 gives the estimated emission of organic compounds from the HLW process cells.

5.2 Potential Emissions Not Considered

The Emission Baseline Report (24590-WTP-RPT-03-008) proposed that the temperature and conditions in the melters and thermal oxidation units are sufficient to generate products of incomplete combustion (PICs) that would be introduced into the offgas streams. The melter offgas containing the PICs will be treated by a melter submerged bed scrubber, which will recycle scrubber liquor back into the pretreatment process. However, the Emission Baseline Report (24590-WTP-RPT-03-008) predicted that PICs recycled to the pretreatment plant will be at concentrations orders-of-magnitude less than the constituent organic compounds. Thus, PICs were not included as emissions in this calculation.

6 References

6.1 Codes and Standards

EPA 1995. *Protocol for Equipment Leak Emission Estimates*, EPA-453/R-95-017. November 1995. US Environmental Protection Agency, Research Triangle Park, North Carolina, USA.

EPA 1998. *Human Health Risk Assessment Protocol*, EPA530-D-98-001A. July 1998. US Environmental Protection Agency, Research Triangle Park, North Carolina, USA.

WAC 173-400. *General Regulations for Air Pollution Sources*, as amended. Washington Administrative Code.

6.2 Project Documents

24590-LAW-RPT-ENG-01-001, Rev. 0, *LAW Vitrification Capacity and Availability Study*.

CCN 023430, Meeting Minutes from 9/6/2001 and 9/7/2001 Meeting with the following purpose: "Discuss Proposed Final Resolution of Remaining Open Comments on the Risk Assessment Work Plan, Item 27.

CCN 068045, E-mail message from Ian Tanner to John Sipkowski, 28 May 2003, "Jumper Breakdown for Environmental Risk Assessment."

CCN 068046, E-mail message from Steven Cross to John Sipkowski, 28 May 2003, "Jumper Counts – Slurry Carrying Jumpers."

CCN 068047, E-mail message from Connie Feuz to John Sipkowski, 4 June 2003, "Connector Count."

PIL-4.08.06, Plant Item List, September, 2001.

24590-WTP-RPT-PO-03-008, Rev. 0, *Integrated Emissions Baseline Report for the Hanford Tank Waste Treatment and Immobilization Plant*.

RPT-24590-EN00003, Rev. 0, *RPP-WTP Waste Feed Assessment*.

Appendix A

Excel Worksheets:

Table 1. Estimate of the Release of Organic Compounds from Ancillary Equipment A-1

Table 2. Post-Evaporator Concentration and Henry's Law Grouping A-2

Table 3. LAW Stream Concentration and Henry's Law Grouping A-3

Table 4. HLW Stream Concentration and Henry's Law Grouping A-4

Table 5. Estimate of Organic Emissions from the Pretreatment Feed Stream A-5

Table 6. Estimate of Organic Emissions from the Post-Evaporator Stream A-9

Table 7. Estimate of Organic Emissions from Pretreatment Process Cells A-14

Table 8. Estimate of Organic Emissions from the LAW Process Cells A-20

Table 9. Estimate of Organic Emissions from the HLW Process Cells A-25

The *Protocol for Equipment Lead Emission Estimates* (EPA 1995) provides the following formula to calculate the estimated release of organic material from ancillary equipment.

$E_{HO} = N \times R_{avg} \times WF_S \times H$, where:

E_{HO} = estimated annual release, kg/year

N = ancillary equipment count by equipment type; equipment count was obtained form Melter Systems group, Area Plant Design, and the Plant Item List (PIL-4.08.06)

R_{avg} = average release factor by equipment type, (kg/hour); from *Protocol for Equipment Leak Emission Estimates* (EPA 1995)

WF_S = weight fraction of organic material = WFs from tables 5, 6, 8, and 9 for Pretreatment Feed Stream, Post-Evaporator Stream, LAW Stream, and HLW Stream respectively * 1/(1000*1000) to convert from mg/kg to kg/kg

$ER_O = E_{HO}$ kg/yr * 1000 gm/kg / (365 d/yr * 24 hr/d *60 min/hr * 60 s/min) where:

ER_O = waste stream organic release (gm/s) by equipment type

$ER_{O\text{-}PTF}$ = sum of Pretreatment Feed Stream estimated release = Sum ER_O by equipment type

$ER_{O\text{-}PE}$ = sum of Post-Evaporator Stream estimated release = Sum ER_O by equipment type

$ER_{O\text{-}LA}$ = sum of LAW Stream estimated release = Sum ER_O by equipment type

$ER_{O\text{-}HL}$ = sum of HLW Stream estimated release = Sum ER_O by equipment type

Table 1. Estimate of the Release of Organic Compounds from Ancillary Equipment. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

Plant	Waste Stream	Equipment Type	Count N	R_{avg} (kg/hour)	Waste Stream Organic Weight Fraction WF_S	Operating Hours H hr/yr	Estimated Annual Release E_{HO} (kg/yr)	Estimated Release ER_O (gm/s)
Pretreatment	Pretreatment Feed Stream	Valves	15	0.00023	0.0083839	8760	0.2534	8.04E-06
		Connectors	170	0.00183	0.0083839	8760	22.8482	7.25E-04
	Pretreatment Feed Stream Total $ER_{O\text{-}PTF}$ =							**7.33E-04**
	Post-Evaporator Stream	Valves	355	0.00023	0.0014825	8760	1.0604	3.36E-05
		Connectors	978	0.00183	0.0014825	8760	23.2426	7.37E-04
	Post-Evaporator Stream Total $ER_{O\text{-}PE}$ =							**7.71E-04**
LAW	LAW Stream	Valves	32	0.00023	0.002454995	8760	0.1583	5.02E-06
		Connectors	44	0.00183	0.002454995	8760	1.7316	5.49E-05
	LAW Stream Total $ER_{O\text{-}LA}$ =							**5.99E-05**
HLW	HLW Stream	Valves	26	0.00023	0.0010959	8760	0.0574	1.82E-06
		Connectors	48	0.00183	0.0010959	8760	0.8432	2.67E-05
	HLW Stream Total $ER_{O\text{-}HL}$ =							**2.85E-05**

CF_{PE} = 60 sec/min x 1/ Q_V ft^3/min x 35.315 ft^3/1000 L x 1000 mg/L x ρ kg/L = Concentration mg/kg

CF_{PE} = Conversion Factor

Q_V = Volumetric Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet FEP03 = 1.19E+00 ft^3/min

ρ = Density from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet FEP03 = 1.50E+00 kg/L

Note: Un-rounded values for Q_V and ρ rom Sheet FET03 were used for the calculations.

CF_{PE} = 1190.702384

Q_M = Compound Mass Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet FEP03

WF_i = Weight Fraction = Q_M * CF_{PE}

Average Weight Fraction WF_a = average WF_i for Henry's Law Group

Table 2. Post-Evaporator Concentration and Henry's Law Grouping. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

Compound CAS#	Organic Compounds	Compound Mass Flow Rate Q_M g/s	Individual Organic Weight Fraction. WF_i mg/kg	Henry's Law Grouping HL	Henry's Law Group Average Organic Weight Fraction. WF_a mg/kg
100-21-0	p-Phthalic acid	4.82E-02	5.74E+01	1	5.74E+01
88-89-1	Picric acid	5.99E-02	7.13E+01	2	7.13E+01
144-62-7	Oxalic acid	4.83E-03	5.75E+00	3	5.75E+00
75-12-7	Formamide	4.80E-02	5.72E+01	4	5.72E+01
60-35-5	Acetamide	1.05E-02	1.24E+01	5	1.24E+01
87-86-5	Pentachlorophenol	4.63E-02	5.51E+01	6	5.51E+01
126-73-8	Tributyl phosphate	3.81E-02	4.54E+01	7	4.54E+01
108-95-2	Phenol	3.00E-02	3.57E+01	8	3.49E+01
84-66-2	Diethyl phthalate	2.24E-02	2.67E+01	8	3.49E+01
88-85-7	2-sec-Butyl-4,6-dinitrophenol (Dinoseb)	3.55E-02	4.23E+01	8	3.49E+01
62-75-9	N-Nitroso-N,N-dimethylamine	1.94E-02	2.31E+01	9	2.31E+01
122-39-4	N,N-Diphenylamine	1.33E-03	1.58E+00	10	8.11E-01
8001-35-2	Toxaphene	3.50E-05	4.17E-02	10	8.11E-01
4170-30-3	2-Butenaldehyde (2-Butenal)	4.69E-04	5.58E-01	11	1.90E+00
58-90-2	2,3,4,6-Tetrachlorophenol	2.34E-03	2.78E+00	11	1.90E+00
98-86-2	Acetophenone	1.98E-03	2.36E+00	11	1.90E+00
57-14-7	1,1-Dimethylhydrazine	1.63E-03	1.94E+00	12	1.94E+00
120-12-7	Anthracene	2.62E-04	3.12E-01	13	2.49E-01
75-05-8	Acetonitrile	1.56E-04	1.86E-01	13	2.49E-01
208-96-8	Acenaphthylene	8.79E-05	1.05E-01	14	1.05E-01
132-64-9	Dibenzofuran	2.88E-05	3.43E-02	15	3.43E-02
106-93-4	Ethylene dibromide (Dibromethane)	2.80E-06	3.33E-03	16	1.33E-03
76-44-8	Heptachlor	3.29E-07	3.92E-04	16	1.33E-03
91-20-3	Naphthalene	2.25E-07	2.68E-04	16	1.33E-03
120-82-1	1,2,4-Trichlorobenzene	1.08E-07	1.29E-04	17	1.29E-04
118-74-1	Hexachlorobenzene	6.76E-09	8.05E-06	18	8.05E-06
10061-01-5	cis-1,3-Dichloropropene	2.16E-08	2.57E-05	19	1.06E-05
108-88-3	Toluene	1.94E-09	2.31E-06	19	1.06E-05
71-43-2	Benzene	3.19E-09	3.80E-06	19	1.06E-05
79-01-6	Trichloroethylene	6.57E-10	7.82E-07	20	7.31E-07
87-68-3	Hexachlorobutadiene	5.70E-10	6.79E-07	20	7.31E-07
127-18-4	Perchloroethylene (tetrachloroethylene)	1.20E-10	1.43E-07	21	1.43E-07
56-23-5	Carbon tetrachloride	3.25E-11	3.86E-08	22	3.86E-08
106-99-0	1,3-Butadiene	1.78E-12	2.12E-09	23	2.12E-09
110-82-7	Cyclohexane	2.13E-13	2.53E-10	24	2.53E-10
108-87-2	Methylcyclohexane	9.07E-15	1.08E-11	25	1.08E-11
106-97-8	Butane	8.13E-16	9.68E-13	26	9.68E-13
110-54-3	n-Hexane	1.23E-16	1.47E-13	27	1.47E-13
111-84-2	n-Nonane	1.86E-17	2.22E-14	28	2.22E-14
76-15-3	Chloropentafluoroethane	4.19E-18	4.99E-15	29	4.99E-15
319-85-7	Hexachlorocyclohexane (Lindane) Beta BHC	1.16E-04	1.38E-01	30	3.21E-01
50-32-8	Benzo(a)pyrene	4.23E-04	5.04E-01	30	3.21E-01
84-74-2	Dibutyl phthalate	1.29E-02	1.53E+01	31	1.53E+01
218-01-9	Chrysene	4.88E-03	5.81E+00	32	3.47E+00
58-89-9	gamma-BHC (Lindane)	1.73E-05	2.06E-02	32	3.47E+00
603-34-9	Triphenylamine	3.84E-03	4.57E+00	32	3.47E+00
129-00-0	Pyrene	2.21E-03	2.63E+00	33	1.33E+00
60-57-1	Dieldrin	1.86E-05	2.21E-02	33	1.33E+00
309-00-2	Aldrin	7.54E-06	8.98E-03	34	8.98E-03
1336-36-3	Polychlorinated biphenyls (PCBs)	5.01E-05	5.97E-02	35	5.97E-02

CF_{LA} = 60 sec/min x 1/ Q_V ft^3/min x 35.315 ft^3/1000 L x 1000 mg/L x ρ kg/L = Concentration mg/kg
CF_{LA} = Conversion Factor
Q_V = Volumetric Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet TCP03 = 4.24E-01 ft^3/min
ρ = Density from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet TCP03 = 1.76E+00 kg/L
Note. Un-rounded values for Q_V and ρ rom Sheet TCP03 were used for the calculations.
CF_{LA} = 2835.87806

Q_M = Compound Mass Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet FEP03
WF_i = Weight Fraction = Q_M * CF_{LA}
Average Weight Fraction WF_a = average WF_i for Henry's Law Group

Table 3. LAW Stream Concentration and Henry's Law Grouping. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

Compound CAS#	Organic Compounds	Compound Mass Flow Rate Q_m g/s	Individual Organic Weight Fraction. WF_i mg/kg	Henry's Law Grouping HL	Henry's Law Group Average Organic Weight Fraction. WF_a mg/kg
100-21-0	p-Phthalic acid	2.73E-02	77.48	1	7.75E+01
88-89-1	Picric acid	3.64E-01	1032.27	2	1.03E+03
144-62-7	Oxalic acid	2.73E-03	7.73	3	7.73E+00
75-12-7	Formamide	2.72E-02	77.05	4	7.71E+01
60-35-5	Acetamide	5.81E-03	16.47	5	1.65E+01
87-86-5	Pentachlorophenol	2.50E-02	70.99	6	7.10E+01
126-73-8	Tributyl phosphate	1.67E-02	47.44	7	4.74E+01
108-95-2	Phenol	1.04E-02	29.37	8	3.48E+01
84-66-2	Diethyl phthalate	5.83E-03	16.54	8	3.48E+01
88-85-7	2-sec-Butyl-4,6-dinitrophenol (Dinoseb)	2.06E-02	58.53	8	3.48E+01
62-75-9	N-Nitroso-N,N-dimethylamine	2.42E-03	6.86	9	6.86E+00
122-39-4	N,N-Diphenylamine	9.65E-05	0.27	10	1.38E-01
8001-35-2	Toxaphene	9.31E-07	0.00	10	1.38E-01
4170-30-3	2-Butenaldehyde (2-Butenal)	1.28E-05	0.04	11	1.24E-01
58-90-2	2,3,4,6-Tetrachlorophenol	6.86E-05	0.19	11	1.24E-01
98-86-2	Acetophenone	4.94E-05	0.14	11	1.24E-01
57-14-7	1,1-Dimethylhydrazine	3.45E-05	0.10	12	9.79E-02
120-12-7	Anthracene	9.40E-07	0.00	13	2.71E-03
75-05-8	Acetonitrile	9.73E-07	0.00	13	2.71E-03
208-96-8	A	1.13E-07	0.00	14	3.20E-04
132-64-9	Dibenzofuran	5.68E-09	0.00	15	1.61E-05
106-93-4	Ethylene dibromide (Dibromethane)	1.12E-11	0.00	16	1.06E-08
76-44-8	Heptachlor	0.00E+00	0.00	16	1.06E-08
91-20-3	Naphthalene	0.00E+00	0.00	16	1.06E-08
120-82-1	1,2,4-Trichlorobenzene	0.00E+00	0.00	17	0.00E+00
118-74-1	Hexachlorobenzene	0.00E+00	0.00	18	0.00E+00
10061-01-5	cis-1,3-Dichloropropene	0.00E+00	0.00	19	0.00E+00
108-88-3	Toluene	0.00E+00	0.00	19	0.00E+00
71-43-2	Benzene	0.00E+00	0.00	19	0.00E+00
79-01-6	Trichloroethylene	0.00E+00	0.00	20	0.00E+00
87-68-3	Hexachlorobutadiene	0.00E+00	0.00	20	0.00E+00
127-18-4	Perchloroethylene (tetrachloroethylene)	0.00E+00	0.00	21	0.00E+00
56-23-5	Carbon tetrachloride	0.00E+00	0.00	22	0.00E+00
106-99-0	1,3-Butadiene	0.00E+00	0.00	23	0.00E+00
110-82-7	Cyclohexane	0.00E+00	0.00	24	0.00E+00
108-87-2	Methylcyclohexane	0.00E+00	0.00	25	0.00E+00
106-97-8	Butane	0.00E+00	0.00	26	0.00E+00
110-54-3	n-Hexane	0.00E+00	0.00	27	0.00E+00
111-84-2	n-Nonane	0.00E+00	0.00	28	0.00E+00
76-15-3	Chloropentafluoroethane	0.00E+00	0.00	29	0.00E+00
319-85-7	Hexachlorocyclohexane (Lindane) Beta BHC	3.42E-05	0.10	30	2.39E-01
50-32-8	Benzo(a)pyrene	1.34E-04	0.38	30	2.39E-01
84-74-2	Dibutyl phthalate	2.02E-03	5.73	31	5.73E+00
218-01-9	Chrysene	2.64E-04	0.75	32	4.21E-01
58-89-9	gamma-BHC (Lindane)	5.41E-07	0.00	32	4.21E-01
603-34-9	Triphenylamine	1.81E-04	0.51	32	4.21E-01
129-00-0	Pyrene	4.99E-05	0.14	33	7.11E-02
60-57-1	Dieldrin	2.65E-07	0 00	33	7.11E-02
309-00-2	Aldrin	1 30E-08	0.00	34	3.67E-05
1336-36-3	Polychlorinated biphenyls (PCBs)	6.02E-11	0.00	35	1.71E-07

CF_{HL} = 60 sec/min x 1/ Q_V ft^3/min x 35.315 ft^3/1000 L x 1000 mg/L x 1 ρ kg/L = Concentration mg/kg

CF_{HL} = Conversion Factor

Q_V = Volumetric Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet HLP09 = 7.65E-01 ft^3/min

ρ : Density from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet HLP09 = 1.04E+00 kg/L

Note Un-rounded values for QV and ρ from Sheet HLP09 were used for the calculations.

CF_{HL} = 2652.33539

Q_M = Compound Mass Flow Rate from the Emission Baseline Report (24590-WTP-RPT-PO-03-008), Sheet FEP03

WF_i = Weight Fraction = Q_M * CF_{HL}

Average Weight Fraction WF_a = average WF_i for Henry's Law Group

Table 4. HLW Stream Concentration and Henry's Law Grouping. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

Compound CAS#	Organic Compounds	Compound Mass Flow Rate Q_m g/s	Individual Organic Weight Fraction. WF_i mg/kg	Henry's Law Grouping HL	Henry's Law Group Average Organic Weight Fraction. WF_a mg/kg
100-21-0	p-Phthalic acid	7.49E-03	19.87	1	1.99E+01
88-89-1	Picric acid	9.30E-03	24.68	2	2.47E+01
144-62-7	Oxalic acid	7.51E-04	1.99	3	1.99E+00
75-12-7	Formamide	7.48E-03	19.85	4	1.98E+01
60-35-5	Acetamide	1.66E-03	4.40	5	4.40E+00
87-86-5	Pentachlorophenol	7.54E-03	20.00	6	2.00E+01
126-73-8	Tributyl phosphate	7.59E-03	20.14	7	2.01E+01
108-95-2	Phenol	7.39E-03	19.59	8	2.21E+01
84-66-2	Diethyl phthalate	6.97E-03	18.48	8	2.21E+01
88-85-7	2-sec-Butyl-4,6-dinitrophenol (Dinoseb)	1.07E-02	28.29	8	2.21E+01
62-75-9	N-Nitroso-N,N-dimethylamine	1.09E-02	28.81	9	2.88E+01
122-39-4	N,N-Diphenylamine	1.14E-03	3.02	10	1.57E+00
8001-35-2	Toxaphene	4.52E-05	0.12	10	1.57E+00
4170-30-3	2-Butenaldehyde (2-Butenal)	8.77E-04	2.33	11	7.83E+00
58-90-2	2,3,4,6-Tetrachlorophenol	4.09E-03	10.85	11	7.83E+00
98-86-2	Acetophenone	3.89E-03	10.32	11	7.83E+00
57-14-7	1,1-Dimethylhydrazine	3.65E-03	9.67	12	9.67E+00
120-12-7	Anthracene	1.23E-03	3.28	13	2.48E+00
75-05-8	Acetonitrile	6.35E-04	1.69	13	2.48E+00
208-96-8	Acenaphthylene	3.94E-04	1.05	14	1.05E+00
132-64-9	Dibenzofuran	9.06E-05	0.24	15	2.40E-01
106-93-4	Ethylene dibromide (Dibromethane)	2.33E-06	0.01	16	3.04E-03
76-44-8	Heptachlor	7.72E-07	0.00	16	3.04E-03
91-20-3	Naphthalene	3.32E-07	0.00	16	3.04E-03
120-82-1	1,2,4-Trichlorobenzene	2.66E-08	0.00	17	7.06E-05
118-74-1	Hexachlorobenzene	1.22E-09	0.00	18	3.23E-06
10061-01-5	cis-1,3-Dichloropropene	1.66E-09	0.00	19	1.55E-06
108-88-3	Toluene	2.73E-11	0.00	19	1.55E-06
71-43-2	Benzene	6.36E-11	0.00	19	1.55E-06
79-01-6	Trichloroethylene	4.37E-12	0.00	20	1.03E-08
87-68-3	Hexachlorobutadiene	3.44E-12	0.00	20	1.03E-08
127-18-4	Perchloroethylene (tetrachloroethylene)	2.48E-13	0.00	21	6.57E-10
56-23-5	Carbon tetrachloride	2.75E-14	0.00	22	7.29E-11
106-99-0	1,3-Butadiene	2.11E-16	0.00	23	5.60E-13
110-82-7	Cyclohexane	1.24E-24	0.00	24	3.30E-21
108-87-2	Methylcyclohexane	0.00E+00	0.00	25	0.00E+00
106-97-8	Butane	0.00E+00	0.00	26	0.00E+00
110-54-3	n-Hexane	0.00E+00	0.00	27	0.00E+00
111-84-2	n-Nonane	0.00E+00	0.00	28	0.00E+00
76-15-3	Chloropentafluoroethane	0 00E+00	0.00	29	0.00E+00
319-85-7	Hexachlorocyclohexane (Lindane) Beta BHC	3 15E-05	0.08	30	1.97E-01
50-32-8	Benzo(a)pyrene	1.17E-04	0.31	30	1.97E-01
84-74-2	Dibutyl phthalate	7.33E-03	19.45	31	1.94E+01
218-01-9	Chrysene	5.79E-03	15.36	32	9.24E+00
58-89-9	gamma-BHC (Lindane)	1.99E-05	0.05	32	9.24E+00
603-34-9	Triphenylamine	4.65E-03	12.32	32	9.24E+00
129-00-0	Pyrene	4.82E-03	12.79	33	6.44E+00
60-57-1	Dieldrin	3.51E-05	0.09	33	6.44E+00
309-00-2	Aldrin	3.35E-05	0.09	34	8.88E-02
1336-36-3	Polychlorinated biphenyls (PCBs)	7.98E-05	0.21	35	2.12E-01

C_O = organic concentration; values are from the RPP-WTP Waste Feed Assessment (RPT-24590-EN00003)
ρ = density; values are from RPP-WTP Waste Feed Assessment (RPT-24590-EN00003)
$WF_i = C_O / \rho$
WF_i = the weight fraction of the individual organic compound
WF_S = Sum WF_i
WR_i = the ratio of the individual organic compound weight fraction to the sum of the individual weight fraction = WFi / WF_S
WR_S = Sum WR_i
$R_{IO} = WR_i * ER_{O\text{-}PTF}$; $ER_{O\text{-}PTF}$ is from Table 1
R_{VO} = vapor emissions; R_{VO} is "0" if the compound is a particle or is particle-bound
P = particle; cell has an "X" if the compound is a particle or is particle-bound

Table 5. Estimate of Organic Emissions from the Pretreatment Feed Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compounds	Organic Conc. C_O mg/L	Density ρ kg/L	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
100-00-5	p-Nitrochlorobenzene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
100-21-0	p-Phthalic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
100-25-4	1,4-Dinitrobenzene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
100-41-4	Ethyl benzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
100-42-5	Styrene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
10061-01-5	cis-1,3-Dichloropropene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
10061-02-6	trans-1,3-Dichloropropene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
101-55-3	4-Bromophenylphenyl ether	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
101-84-8	Diphenyl ether	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-35-4	3-Heptanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-42-3	p-Xylene (Dimethyl benzene)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-46-7	1,4-Dichlorobenzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-88-7	1,2-Epoxybutane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-93-4	Ethylene dibromide (Dibromethane)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
106-97-8	Butane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
106-99-0	1,3-Butadiene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-02-8	Acrolein	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-05-1	3-Chloropropene (Allyl chloride)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-06-2	1,2-Dichloroethane (Ethylene chloride)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-12-0	Propionitrile	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-13-1	Acrylonitrile	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
107-18-6	2-Propene-1-ol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
107-31-3	Formic acid, methyl ester	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
107-66-4	Dibutylphosphate	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
107-87-9	2-Pentanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-03-2	1-Nitropropane	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
108-05-4	Vinyl acetate	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-20-3	Bis(isopropyl)ether	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-38-3	m-Xylene (Dimethyl benzene)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-39-4	m-Cresol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-87-2	Methylcyclohexane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-88-3	Toluene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-90-7	Chlorobenzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-93-0	Cyclohexanol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-94-1	Cyclohexanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
108-95-2	Phenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
109-66-0	n-Pentane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
109-99-9	Tetrahydrofuran	39.6	1.35	29.3	3.50E-03	2.57E-06	2.57E-06	
110-12-3	5-Methyl-2-hexanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
110-43-0	2-Heptanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
110-54-3	n-Hexane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
110-62-3	n-Valeraldehyde	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
110-82-7	Cyclohexane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
110-83-8	Cyclohexene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
110-86-1	Pyridine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
111-65-9	n-Octane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
111-76-2	Ethylene glycol monobutyl ether	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
111-84-2	n-Nonane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
117-84-0	n-Dioctyl phthalate	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
118-74-1	Hexachlorobenzene	1.8	1.35	1.3	1.60E-04	1.20E-07	1.20E-07	

Table 5. Estimate of Organic Emissions from the Pretreatment Feed Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compounds	Organic Conc. C_O mg/L	Density ρ kg/L	Individual Organic Weight Fraction. WF, mg/kg	Individual Organic Weight Ratio WR, unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
120-12-7	Anthracene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
120-82-1	1,2,4-Trichlorobenzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
120-83-2	2,4-Dichlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
121-44-8	Triethylamine	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
121-69-7	Dimethylaniline	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
122-39-4	N,N-Diphenylamine	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
123-19-3	4-Heptanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
123-38-6	n-Propionaldehyde	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
123-51-3	3-Methyl-1-butanol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
123-86-4	Acetic acid n-butyl ester	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
123-91-1	1,4-Dioxane	50.9	1.35	37.7	4.50E-03	3.30E-06	3.30E-06	
126-73-8	Tributyl phosphate	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
127-18-4	Perchloroethylene (tetrachloroethylene)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
127-19-5	N,N-Dimethylacetamide	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
129-00-0	Pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
1321-64-8	Pentachloronaphthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
1321-65-9	Trichloronaphthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
132-64-9	Dibenzofuran	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
1335-87-1	Hexachloronaphthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
1335-88-2	Tetrachloronaphthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
1336-36-3	Polychlorinated biphenyls (PCBs)	29.4	1.35	21.8	2.60E-03	1.91E-06	0.00E+00	X
141-78-6	Acetic acid ethyl ester (Ethyl acetate)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
141-79-7	4-Methyl-3-penten-2-one	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
142-82-5	n-Heptane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
144-62-7	Oxalic acid	8.5	1.35	6.3	7.50E-04	5.50E-07	5.50E-07	
156-60-5	trans-1,2-Dichloroethylene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
1582-09-8	Trifluralin	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
1634-04-4	Methyl tert-butyl ether	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
1836-75-5	Nitrofen	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
189-55-9	Dibenzo[a,i]pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
189-64-0	Dibenzo[a,h]pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
191-24-2	Benzo(g,h,i)perylene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
191-30-0	Benzo[a,i]pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
192-65-4	Dibenzo[a,e]pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
193-39-5	Indeno(1,2,3-cd)pyrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
205-82-3	Benzo(j)fluoranthene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
205-99-2	Benzo(b)fluoranthene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
206-44-0	Fluoranthene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
207-08-9	Benzo(k)fluoranthene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
208-96-8	Acenaphthylene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
218-01-9	Chrysene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
2234-13-1	Octachloronaphthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
224-42-0	Dibenz[a,j]acridine	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
226-36-8	Dibenz[a,h]acridine	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
2385-85-5	Mirex	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
25551-13-7	Trimethyl benzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
26140-60-3	Terphenyls	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
27154-33-2	Trichlorofluoroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
287-92-3	Cyclopentane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
309-00-2	Aldrin	1	1.35	0.7	9.00E-05	7.00E-08	0.00E+00	X
319-84-6	Hexachlorocyclohexane (Lindane) Alpha BHC	0.3	1.35	0.2	3.00E-05	2.00E-08	2.00E-08	
319-85-7	Hexachlorocyclohexane (Lindane) Beta BHC	0.3	1.35	0.2	3.00E-05	2.00E-08	0.00E+00	X
319-86-8	Delta-BHC	0.3	1.35	0.2	3.00E-05	2.00E-08	0.00E+00	X
3697-24-3	5-Methylchrysene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
3825-26-1	Ammonium perfluorooctanoate	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
4170-30-3	2-Butenaldehyde (2-Butenal)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
465-73-6	Isodrin	0.6	1.35	0.4	5.00E-05	4.00E-08	4.00E-08	
50-00-0	Formaldehyde	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
50-29-3	4,4-DDT	0.6	1.35	0.4	5.00E-05	4.00E-08	0.00E+00	X
50-32-8	Benzo(a)pyrene	1.1	1.35	0.8	1.00E-04	7.00E-08	0.00E+00	X
53-70-3	Dibenzo(a,h)anthracene	0.1	1.35	0.1	1.00E-05	1.00E-08	0.00E+00	X
540-59-0	1,2-Dichloroethylene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	

Table 5. Estimate of Organic Emissions from the Pretreatment Feed Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compounds	Organic Conc. C_O mg/L	Density ρ kg/L	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
540-84-1	2,2,4-Trimethylpentane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
541-73-1	1,3-Dichlorobenzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
56-23-5	Carbon tetrachloride	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
563-80-4	3-Methyl-2-butanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
56-49-5	3-Methylcholanthrene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
56-55-3	Benzo(a)anthracene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
57-14-7	1,1-Dimethylhydrazine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
58-89-9	gamma-BHC (Lindane)	0.3	1.35	0.2	3.00E-05	2.00E-08	0.00E+00	X
58-90-2	2,3,4,6-Tetrachlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
591-78-6	2-Hexanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
59-50-7	4-Chloro-3-methylphenol	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
59-89-2	N-Nitrosomorpholine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
602-87-9	5-Nitroacenaphthene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
60-29-7	Ethyl ether	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
603-34-9	Triphenylamine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
60-34-4	Methylhydrazine	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
60-35-5	Acetamide	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
60-57-1	Dieldrin	0.6	1.35	0.4	5.00E-05	4.00E-08	0.00E+00	X
621-64-7	Di-n-Propylnitrosamine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
624-83-9	Methyl isocyanate	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
627-13-4	Nitric acid, propyl ester	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
62-75-9	N-Nitroso-N,N-dimethylamine	158.4	1.35	117.3	1.40E-02	1.03E-05	1.03E-05	
630-20-6	1,1,1,2-Tetrachloroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
64-17-5	Ethyl alcohol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
64-18-6	Formic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
64-19-7	Acetic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
67-56-1	Methyl alcohol (Methanol)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
67-63-0	2-Propyl alcohol (Isopropanol)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
67-64-1	2-Propanone (Acetone)	101.8	1.35	75.4	8.99E-03	6.59E-06	6.59E-06	
67-66-3	Chloroform	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
67-72-1	Hexachloroethane	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
684-16-2	Hexafluoroacetone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
71-23-8	n-Propyl alcohol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
71-36-3	n-Butyl alcohol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
71-43-2	Benzene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
72-20-8	Endrin	0.6	1.35	0.4	5.00E-05	4.00E-08	0.00E+00	X
72-43-5	Methoxychlor	2.8	1.35	2.1	2.50E-04	1.80E-07	0.00E+00	X
72-54-8	4,4-DDD	0.6	1.35	0.4	5.00E-05	4.00E-08	0.00E+00	X
72-55-9	4,4-DDE	0.6	1.35	0.4	5.00E-05	4.00E-08	0.00E+00	X
74-83-9	Bromomethane (Methyl bromide)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
74-87-3	Chloromethane (Methyl chloride)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
74-97-5	Bromochloromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
74-99-7	Methylacetylene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-00-3	Chloroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-01-4	Vinyl chloride (1-Chloroethene)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-05-8	Acetonitrile	26.6	1.35	19.7	2.35E-03	1.72E-06	1.72E-06	
75-07-0	Acetaldehyde	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-09-2	Dichloromethane (Methylene chloride)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-12-7	Formamide	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-15-0	Carbon disulfide	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-21-8	Ethylene oxide (Oxirane)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-27-4	Bromodichloromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-34-3	1,1-Dichloroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-35-4	1,1-Dichloroethene (Vinylidene chloride)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-43-4	Dichlorofluoromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-45-6	Chlorodifluoromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-50-3	Trimethylamine	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-52-5	Nitromethane	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-55-8	2-Methylaziridine	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
75-61-6	Difluorodibromomethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-63-8	Trifluorobromomethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-65-0	2-Methyl-2-propanol	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-69-4	Trichlorofluoromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	

Table 5. Estimate of Organic Emissions from the Pretreatment Feed Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compounds	Organic Conc. C_O mg/L	Density ρ kg/L	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
75-71-8	Dichlorodifluoromethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
75-99-0	2,2-Dichloropropionic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
76-03-9	Trichloroacetic acid	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
76-11-9	1,1,1,2-Tetrachloro-2,2-difluoroethane	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
76-12-0	1,1,2,2-Tetrachloro-1,2-difluoroethane	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
76-13-1	1,2,2-Trichloro-1,1,2-trifluoroethane (Freon 113)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
76-15-3	Chloropentafluoroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
76-44-8	Heptachlor	1.8	1.35	1.3	1.60E-04	1.20E-07	1.20E-07	
78-83-1	2-Methylpropyl alcohol (Isobutyl alcohol)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
78-87-5	1,2-Dichloropropane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
78-92-2	1-Methylpropyl alcohol (2-Butanol)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
78-93-3	Methyl ethyl ketone (MEK, 2-Butanone)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
79-00-5	1,1,2-Trichloroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
79-01-6	Trichloroethylene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
79-09-4	Propionic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
79-10-7	2-Propenoic acid	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
79-20-9	Methyl acetate	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
79-34-5	1,1,2,2-Tetrachloroethane	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
8001-35-2	Toxaphene	0.7	1.35	0.5	6.00E-05	4.00E-08	0.00E+00	X
82-68-8	Pentachloronitrobenzene (PCBN)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
83-32-9	Acenaphthene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
84-66-2	Diethyl phthalate	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
84-74-2	Dibutyl phthalate	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
85-01-8	Phenanthrene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
85-68-7	Butylbenzyl phthalate	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
86-73-7	Fluorene	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
87-68-3	Hexachlorobutadiene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
87-86-5	Pentachlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
88-06-2	2,4,6-Trichlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
88-72-2	2-Nitrotoluene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
88-75-5	2-Nitrophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
88-85-7	2-sec-Butyl-4,6-dinitrophenol (Dinoseb)	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
88-89-1	Picric acid	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
91-20-3	Naphthalene	2.8	1.35	2.1	2.50E-04	1.80E-07	1.80E-07	
91-22-5	Quinoline	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
91-58-7	2-Chloronapthalene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
92-52-4	1,1'-Biphenyl	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
92-93-3	4-Nitrobiphenyl	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
93-72-1	Silvex (2,4,5-TP)	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
93-76-5	2,4,5-T	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
94-75-7	2,4-D and esters (160C typed)	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
95-13-6	Indene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
95-47-6	o-Xylene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
95-48-7	o-Cresol (2-Methylphenol)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
95-49-8	2-Chlorotoluene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
95-50-1	o-Dichlorobenzene (1,2-Dichlorobenzene)	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
95-57-8	2-Chlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
95-95-4	2,4,5-Trichlorophenol	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
96-22-0	3-Pentanone	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
96-69-5	Bis(3-tert-butyl-4-hydroxy-6-methyl-phenyl)sulfide	84.8	1.35	62.8	7.49E-03	5.49E-06	0.00E+00	X
98-51-1	p-tert-Butyltoluene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
98-82-8	Cumene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
98-83-9	alpha-Methylstyrene	18.7	1.35	13.9	1.65E-03	1.21E-06	1.21E-06	
98-86-2	Acetophenone	84.8	1 35	62.8	7.49E-03	5.49E-06	5.49E-06	
98-95-3	Nitrobenzene	84.8	1.35	62.8	7.49E-03	5.49E-06	5.49E-06	
			Weight Fraction Sum = WF_S =	8383.9				
			Weight Ratio Sum = WR_S =		1.0			
			Pretreatment Feed Stream Sum = $ER_{O\text{-}PTF}$ =			7.33E-04		
			Pretreatment Feed Stream Vapor Organic Release Sum = R_{VOS} =				5.11E-04	

HL = Henry's Law Groupings; values for HL are from the Emission Baseline Report (23590-WTP-RPT-PO-03-008)
WF_i = the weight fraction of the individual organic compound; values are assigned from Table 2 based on HL
WF_S = Sum WF_i
WR_i = the ratio of the individual organic compound weight fraction to the sum of the individual weight fraction = WFi / WF_S
WR_S = Sum WR_i
R_{IO} = WR_i * ER_{O-PE}; ER_{O-PE} is from Table 1
R_{VO} = vapor emissions; R_{VO} is "0" if the compound is a particle or is particle-bound
R_{VOS} = Sum R_{VOi}
P = particle; cell has an "X" if the compound is a particle or is particle-bound

Table 6. Estimate of Organic Emissions from the Post-Evaporator Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compound	Henry's Law Grouping HL	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
100-00-5	p-Nitrochlorobenzene	10	8.11E-01	5.47E-04	4.00E-07	4.00E-07	
100-21-0	p-Phthalic acid	1	5.74E+01	3.87E-02	2.98E-05	2.98E-05	
100-25-4	1,4-Dinitrobenzene	6	5.51E+01	3.72E-02	2.86E-05	0.00E+00	X
100-41-4	Ethyl benzene	20	7.31E-07	0.00E+00	0.00E+00	0.00E+00	
100-42-5	Styrene	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
10061-01-5	cis-1,3-Dichloropropene	19	2.57E-05	0.00E+00	0.00E+00	0.00E+00	
10061-02-6	trans-1,3-Dichloropropene	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
101-55-3	4-Bromophenylphenyl ether	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
101-84-8	Diphenyl ether	16	1.33E-03	9.00E-07	1.00E-09	1.00E-09	
106-35-4	3-Heptanone	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
106-42-3	p-Xylene (Dimethyl benzene)	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
106-46-7	1,4-Dichlorobenzene	18	8.05E-06	0.00E+00	0.00E+00	0.00E+00	
106-88-7	1,2-Epoxybutane	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
106-93-4	Ethylene dibromide (Dibromethane)	16	3.33E-03	2.20E-06	2.00E-09	2.00E-09	
106-97-8	Butane	26	9.68E-13	0.00E+00	0.00E+00	0.00E+00	
106-99-0	1,3-Butadiene	23	2.12E-09	0.00E+00	0.00E+00	0.00E+00	
107-02-8	Acrolein	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
107-05-1	3-Chloropropene (Allyl chloride)	20	7.31E-07	0.00E+00	0.00E+00	0.00E+00	
107-06-2	1,2-Dichloroethane (Ethylene chloride)	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
107-12-0	Propionitrile	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
107-13-1	Acrylonitrile	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
107-18-6	2-Propene-1-ol	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
107-31-3	Formic acid, methyl ester	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
107-66-4	Dibutylphosphate	5	1.24E+01	8.39E-03	6.47E-06	0.00E+00	X
107-87-9	2-Pentanone	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
108-03-2	1-Nitropropane	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
108-05-4	Vinyl acetate	16	1.33E-03	9.00E-07	1.00E-09	1.00E-09	
108-10-1	Hexone (4-Methyl-2-pentanone or MIBK)	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
108-20-3	Bis(isopropyl)ether	18	8.05E-06	0.00E+00	0.00E+00	0.00E+00	
108-38-3	m-Xylene (Dimethyl benzene)	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
108-39-4	m-Cresol	9	2.31E+01	1.56E-02	1.20E-05	1.20E-05	
108-87-2	Methylcyclohexane	25	1.08E-11	0.00E+00	0.00E+00	0.00E+00	
108-88-3	Toluene	19	2.31E-06	0.00E+00	0.00E+00	0.00E+00	
108-90-7	Chlorobenzene	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
108-93-0	Cyclohexanol	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
108-94-1	Cyclohexanone	11	1.90E+00	1.28E-03	9.87E-07	9.87E-07	
108-95-2	Phenol	8	3.57E+01	2.41E-02	1.86E-05	1.86E-05	
109-66-0	n-Pentane	26	9.68E-13	0.00E+00	0.00E+00	0.00E+00	
109-99-9	Tetrahydrofuran	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
110-12-3	5-Methyl-2-hexanone	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
110-43-0	2-Heptanone	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
110-54-3	n-Hexane	27	1.47E-13	0.00E+00	0.00E+00	0.00E+00	
110-62-3	n-Valeraldehyde	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
110-82-7	Cyclohexane	24	2.53E-10	0.00E+00	0.00E+00	0.00E+00	
110-83-8	Cyclohexene	22	3.86E-08	0.00E+00	0.00E+00	0.00E+00	

Table 6. Estimate of Organic Emissions from the Post-Evaporator Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compound	Henry's Law Grouping HL	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
110-86-1	Pyridine	11	1.90E+00	1.28E-03	9.87E-07	9.87E-07	
111-65-9	n-Octane	28	2.22E-14	0.00E+00	0.00E+00	0.00E+00	
111-76-2	Ethylene glycol monobutyl ether	9	2.31E+01	1.56E-02	1.20E-05	1.20E-05	
111-84-2	n-Nonane	28	2.22E-14	0.00E+00	0.00E+00	0.00E+00	
117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
117-84-0	n-Dioctyl phthalate	32	3.47E+00	2.34E-03	1.80E-06	0.00E+00	X
118-74-1	Hexachlorobenzene	18	8.05E-06	0.00E+00	0.00E+00	0.00E+00	
120-12-7	Anthracene	13	3.12E-01	2.11E-04	1.62E-07	1.62E-07	
120-82-1	1,2,4-Trichlorobenzene	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
120-83-2	2,4-Dichlorophenol	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
121-44-8	Triethylamine	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
121-69-7	Dimethylaniline	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
122-39-4	N,N-Diphenylamine	10	1.58E+00	1.07E-03	8.21E-07	8.21E-07	
123-19-3	4-Heptanone	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
123-38-6	n-Propionaldehyde	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
123-51-3	3-Methyl-1-butanol	12	1.94E+00	1.31E-03	1.01E-06	1.01E-06	
123-86-4	Acetic acid n-butyl ester	16	1.33E-03	9.00E-07	1.00E-09	1.00E-09	
123-91-1	1,4-Dioxane	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
126-73-8	Tributyl phosphate	7	4.54E+01	3.06E-02	2.36E-05	2.36E-05	
126-98-7	2-Methyl-2-propenenitrile (Methacrylonitrile)	16	1.33E-03	9.00E-07	1.00E-09	1.00E-09	
127-18-4	Perchloroethylene (tetrachloroethylene)	21	1.43E-07	0.00E+00	0.00E+00	0.00E+00	
127-19-5	N,N-Dimethylacetamide	5	1.24E+01	8.39E-03	6.47E-06	6.47E-06	
128-37-0	2,6-Bis(tert-butyl)-4-methylphenol	32	3.47E+00	2.34E-03	1.80E-06	1.80E-06	
129-00-0	Pyrene	33	2.63E+00	1.78E-03	1.37E-06	0.00E+00	X
1321-64-8	Pentachloronaphthalene	14	1.05E-01	7.06E-05	5.44E-08	0.00E+00	X
1321-65-9	Trichloronaphthalene	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
132-64-9	Dibenzofuran	15	3.43E-02	2.31E-05	1.78E-08	1.78E-08	
1335-87-1	Hexachloronaphthalene	14	1.05E-01	7.06E-05	5.44E-08	0.00E+00	X
1335-88-2	Tetrachloronaphthalene	15	3.43E-02	2.31E-05	1.78E-08	0.00E+00	X
1336-36-3	Polychlorinated biphenyls (PCBs)	35	5.97E-02	4.03E-05	3.11E-08	0.00E+00	X
141-78-6	Acetic acid ethyl ester (Ethyl acetate)	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
141-79-7	4-Methyl-3-penten-2-one	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
142-82-5	n-Heptane	27	1.47E-13	0.00E+00	0.00E+00	0.00E+00	
144-62-7	Oxalic acid	3	5.75E+00	3.88E-03	2.99E-06	2.99E-06	
156-60-5	trans-1,2-Dichloroethylene	20	7.31E-07	0.00E+00	0.00E+00	0.00E+00	
1582-09-8	Trifluralin	14	1.05E-01	7.06E-05	5.44E-08	0.00E+00	X
1634-04-4	Methyl tert-butyl ether	16	1.33E-03	9.00E-07	1.00E-09	1.00E-09	
1836-75-5	Nitrofen	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
189-55-9	Dibenzo[a,i]pyrene	5	1.24E+01	8.39E-03	6.47E-06	0.00E+00	X
189-64-0	Dibenzo[a,h]pyrene	5	1.24E+01	8.39E-03	6.47E-06	0.00E+00	X
191-24-2	Benzo(g,h,i)perylene	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
191-30-0	Benzo[a,i]pyrene	5	1.24E+01	8.39E-03	6.47E-06	0.00E+00	X
192-65-4	Dibenzo[a,e]pyrene	5	1.24E+01	8.39E-03	6.47E-06	0.00E+00	X
193-39-5	Indeno(1,2,3-cd)pyrene	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
205-82-3	Benzo(j)fluoranthene	7	4.54E+01	3.06E-02	2.36E-05	0.00E+00	X
205-99-2	Benzo(b)fluoranthene	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
206-44-0	Fluoranthene	33	1.33E+00	8.96E-04	6.90E-07	0.00E+00	X
207-08-9	Benzo(k)fluoranthene	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
208-96-8	Acenaphthylene	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
218-01-9	Chrysene	32	5.81E+00	3.92E-03	3.02E-06	0.00E+00	X
2234-13-1	Octachloronaphthalene	14	1.05E-01	7.06E-05	5.44E-08	0.00E+00	X
224-42-0	Dibenz[a,j]acridine	4	5.72E+01	3.86E-02	2.97E-05	0.00E+00	X
226-36-8	Dibenz[a,h]acridine	4	5.72E+01	3.86E-02	2.97E-05	0.00E+00	X
2385-85-5	Mirex	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
25551-13-7	Trimethyl benzene	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
26140-60-3	Terphenyls	34	8.98E-03	6.10E-06	4.70E-09	0.00E+00	X
27154-33-2	Trichlorofluoroethane	23	2.12E-09	0.00E+00	0.00E+00	0.00E+00	

Table 6. Estimate of Organic Emissions from the Post-Evaporator Stream. Calc. No. 24590-WTP-HAC-50-00001, Rev. C

CAS#	Organic Compound	Henry's Law Grouping HL	Individual Organic Weight Fraction. WF_i mg/kg	Individual Organic Weight Ratio WR_i unitless	Individual Organic Release R_{IO} gm/s	Individual Organic Vapor Emission R_{VO} gm/s	Particle P
287-92-3	Cyclopentane	24	2.53E-10	0.00E+00	0.00E+00	0.00E+00	
309-00-2	Aldrin	34	8.98E-03	6.10E-06	4.70E-09	0.00E+00	X
319-84-6	Hexachlorocyclohexane (Lindane) Alpha BHC	33	1.33E+00	8.96E-04	6.90E-07	6.90E-07	
319-85-7	Hexachlorocyclohexane (Lindane) Beta BHC	30	1.38E-01	9.34E-05	7.20E-08	0.00E+00	X
319-86-8	Delta-BHC	30	3.21E-01	2.17E-04	1.67E-07	0.00E+00	X
3697-24-3	5-Methylchrysene	32	3.47E+00	2.34E-03	1.80E-06	0.00E+00	X
3825-26-1	Ammonium perfluorooctanoate	14	1.05E-01	7.06E-05	5.44E-08	0.00E+00	X
4170-30-3	2-Butenaldehyde (2-Butenal)	11	5.58E-01	3.77E-04	2.90E-07	2.90E-07	
465-73-6	Isodrin	35	5.97E-02	4.03E-05	3.11E-08	3.11E-08	
50-00-0	Formaldehyde	8	3.49E+01	2.35E-02	1.81E-05	1.81E-05	
50-29-3	4,4-DDT	33	1.33E+00	8.96E-04	6.90E-07	0.00E+00	X
50-32-8	Benzo(a)pyrene	30	5.04E-01	3.40E-04	2.62E-07	0.00E+00	X
53-70-3	Dibenzo(a,h)anthracene	7	4.54E+01	3.06E-02	2.36E-05	0.00E+00	X
540-59-0	1,2-Dichloroethylene	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
540-84-1	2,2,4-Trimethylpentane	28	2.22E-14	0.00E+00	0.00E+00	0.00E+00	
541-73-1	1,3-Dichlorobenzene	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
56-23-5	Carbon tetrachloride	22	3.86E-08	0.00E+00	0.00E+00	0.00E+00	
563-80-4	3-Methyl-2-butanone	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
56-49-5	3-Methylcholanthrene	28	2.22E-14	0.00E+00	0.00E+00	0.00E+00	X
56-55-3	Benzo(a)anthracene	33	1.33E+00	8.96E-04	6.90E-07	0.00E+00	X
57-14-7	1,1-Dimethylhydrazine	12	1.94E+00	1.31E-03	1.01E-06	1.01E-06	
58-89-9	gamma-BHC (Lindane)	32	2.06E-02	1.39E-05	1.07E-08	0.00E+00	X
58-90-2	2,3,4,6-Tetrachlorophenol	11	2.78E+00	1.88E-03	1.45E-06	1.45E-06	
591-78-6	2-Hexanone	14	1.05E-01	7.06E-05	5.44E-08	5.44E-08	
59-50-7	4-Chloro-3-methylphenol	32	3.47E+00	2.34E-03	1.80E-06	0.00E+00	X
59-89-2	N-Nitrosomorpholine	6	5.51E+01	3.72E-02	2.86E-05	2.86E-05	
602-87-9	5-Nitroacenaphthene	9	2.31E+01	1.56E-02	1.20E-05	0.00E+00	X
60-29-7	Ethyl ether	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
603-34-9	Triphenylamine	32	4.57E+00	3.08E-03	2.37E-06	2.37E-06	
60-34-4	Methylhydrazine	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
60-35-5	Acetamide	5	1.24E+01	8.39E-03	6.47E-06	6.47E-06	
60-57-1	Dieldrin	33	2.21E-02	1.49E-05	1.15E-08	0.00E+00	X
621-64-7	Di-n-Propylnitrosamine	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
624-83-9	Methyl isocyanate	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
627-13-4	Nitric acid, propyl ester	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	
62-75-9	N-Nitroso-N,N-dimethylamine	9	2.31E+01	1.56E-02	1.20E-05	1.20E-05	
630-20-6	1,1,1,2-Tetrachloroethane	18	8.05E-06	0.00E+00	0.00E+00	0.00E+00	
64-17-5	Ethyl alcohol	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
64-18-6	Formic acid	7	4.54E+01	3.06E-02	2.36E-05	2.36E-05	
64-19-7	Acetic acid	6	5.51E+01	3.72E-02	2.86E-05	2.86E-05	
67-56-1	Methyl alcohol (Methanol)	10	8.11E-01	5.47E-04	4.21E-07	4.21E-07	
67-63-0	2-Propyl alcohol (Isopropanol)	11	1.90E+00	1.28E-03	9.90E-07	9.90E-07	
67-64-1	2-Propanone (Acetone)	13	2.49E-01	1.68E-04	1.29E-07	1.29E-07	
67-66-3	Chloroform	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
67-72-1	Hexachloroethane	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
684-16-2	Hexafluoroacetone	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
71-23-8	n-Propyl alcohol	11	1.90E+00	1.28E-03	9.87E-07	9.87E-07	
71-36-3	n-Butyl alcohol	11	1.90E+00	1.28E-03	9.87E-07	9.87E-07	
71-43-2	Benzene	19	3.80E-06	0.00E+00	0.00E+00	0.00E+00	
71-55-6	Methyl chloroform (1,1,1-Trichloroethane)	21	1.43E-07	0.00E+00	0.00E+00	0.00E+00	
72-20-8	Endrin	32	3.47E+00	2.34E-03	1.80E-06	0.00E+00	X
72-43-5	Methoxychlor	7	4.54E+01	3.06E-02	2.36E-05	0.00E+00	X
72-54-8	4,4-DDD	32	3.47E+00	2.34E-03	1.80E-06	0.00E+00	X
72-55-9	4,4-DDE	34	8.98E-03	6.10E-06	5.00E-09	0.00E+00	X
74-83-9	Bromomethane (Methyl bromide)	19	1.06E-05	0.00E+00	0.00E+00	0.00E+00	
74-87-3	Chloromethane (Methyl chloride)	20	7.31E-07	0.00E+00	0.00E+00	0.00E+00	
74-97-5	Bromochloromethane	17	1.29E-04	1.00E-07	0.00E+00	0.00E+00	