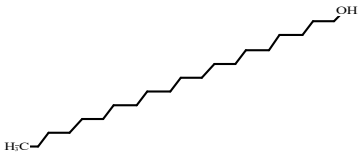
CAS Number: 629-96-9
SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): 8.30
Boiling Point (deg C) : ------
Melting Point (deg C) : 64.00
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



KOWWIN Program (v1.68) Results:
==========

Log Kow(version 1.68 estimate):

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	19	-CH2- [aliphatic carbon]	0.4911	9.3309
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Const		Equation Constant		0.2290
			Log Kow =	8.6986

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match:
Name : 1-EICOSANOL
CAS Num : 000629-96-9
Exp MP (deg C): 66.1
Exp BP (deg C): 372
Exp VP (mm Hg): 4.52E-08 (extrapolated)
(Pa): 6.03E-006
Exp VP (deg C): 25
Exp VP ref : YAWS,CL (1994B)

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 377.87 deg C (Adapted Stein and Brown Method)

Melting Point: 102.82 deg C (Adapted Joback Method)
Melting Point: 106.98 deg C (Gold and Ogle Method)
Mean Melt Pt : 104.90 deg C (Joback; Gold,Ogle Methods)
Selected MP: 104.90 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 372.00 deg C (exp database))
(Using MP: 64.00 deg C (user entered))
VP: 1.44E-007 mm Hg (Antoine Method)
: 1.91E-005 Pa (Antoine Method)
VP: 5.24E-007 mm Hg (Modified Grain Method)
: 6.98E-005 Pa (Modified Grain Method)

```
    VP:  3.27E-005 mm Hg (Mackay Method)
       :  0.00436 Pa  (Mackay Method)
  Selected VP:  5.24E-007 mm Hg (Modified Grain Method)
             :  6.98E-005 Pa (Modified Grain Method)
  Subcooled liquid VP:  1.1E-007 mm Hg (25 deg C, exp database VP )
                     :  1.46E-005 Pa  (25 deg C, exp database VP )

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 19  |  -CH2-             |   24.22  |  460.18
 Group |  1  |  -OH (primary)     |   88.46  |   88.46
   *   |     |  Equation Constant |          |  198.18
============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  768.80
RESULT- corr |  BOILING POINT in deg Kelvin  |  651.03
             |  BOILING POINT in deg C       |  377.87
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 19  |  -CH2-             |   11.27  |  214.13
 Group |  1  |  -OH (primary)     |   44.45  |   44.45
   *   |     |  Equation Constant |          |  122.50
============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  375.98
             |  MELTING POINT in deg C       |  102.82
-------------------------------------------------------



Water Sol from Kow (WSKOW v1.42) Results:
=========================================

          Water Sol: 0.002127 mg/L

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM   : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
---------------------------------- WSKOW v1.42 Results -----------------------
Log Kow  (estimated)  :  8.70
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  8.30 (user entered)

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

      Melting Pt (Tm) = 64.00 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       Alcohol, aliphatic    0.424

   Log Water Solubility  (in moles/L) :  -8.147
   Water Solubility at 25 deg C (mg/L):  0.002127



WATERNT Program (v1.01) Results:
================================

                  Water Sol (v1.01 est): 0.00063219 mg/L

SMILES : CCCCCCCCCCCCCCCCCCCCO
```

CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	19	-CH2- [aliphatic carbon]	-0.5370	-10.2034
Frag	1	-OH [hydroxy, aliphatic attach]	1.6012	1.6012
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -8.6742
Water Solubility (mg/L) at 25 dec C =0.00063219

ECOSAR Program (v1.11) Results:
==========
ECOSAR Version 1.11 Results Page

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
CAS Num:
ChemID1:
MOL FOR: C20 H42 O1
MOL WT : 298.56
Log Kow: 8.699 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: 64.00 (deg C, User Entered for Wat Sol estimate)
Melt Pt: 66.10 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.0008813 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 8.699 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 0.0008813 (mg/L, EPISuite WSKowwin v1.43 Estimate)

ECOSAR v1.11 Class-specific Estimations

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	Fish	96-hr	LC50	0.000236
Neutral Organics	Daphnid	48-hr	LC50	0.000249
Neutral Organics	Green Algae	96-hr	EC50	0.002 *
Neutral Organics	Fish		ChV	4.79e-005
Neutral Organics	Daphnid		ChV	0.000136
Neutral Organics	Green Algae		ChV	0.002 *
Neutral Organics	Fish (SW)	96-hr	LC50	0.00031
Neutral Organics	Mysid	96-hr	LC50	2.46e-006
Neutral Organics	Fish (SW)		ChV	0.002 *
Neutral Organics	Mysid (SW)		ChV	2.92e-008
Neutral Organics	Earthworm	14-day	LC50	104.854 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

```
------------------------------
Class Specific LogKow Cut-Offs
------------------------------
If the log Kow of the chemical is greater than the endpoint specific cut-offs
presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:
----------------
Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
```

```
HENRYWIN (v3.20) Program Results:
=============================

       Bond Est :  9.29E-004 atm-m3/mole  (9.42E+001 Pa-m3/mole)
       Group Est:  2.45E-003 atm-m3/mole  (2.48E+002 Pa-m3/mole)

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM   : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
--------------------------- HENRYWIN v3.20 Results -------------------------
----------+-----------------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION             | COMMENT |  VALUE
----------+-----------------------------------------------+---------+----------
 HYDROGEN |  41  Hydrogen to Carbon (aliphatic) Bonds     |         | -4.9068
 HYDROGEN |   1  Hydrogen to Oxygen Bonds                 |         |  3.2318
 FRAGMENT |  19  C-C                                      |         |  2.2098
 FRAGMENT |   1  C-O                                      |         |  1.0855
 FACTOR   |   *  Non-cyclic alkyl or olefinic alcohol     |         |  -.2000
----------+-----------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE     |  TOTAL  |  1.420
----------+-----------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 9.29E-004 atm-m3/mole
                                = 3.80E-002 unitless
                                = 9.42E+001 Pa-m3/mole

--------+-----------------------------------------------+------------+--------
        |        GROUP CONTRIBUTION DESCRIPTION         |   COMMENT  |  VALUE
--------+-----------------------------------------------+------------+--------
        |           1  CH3 (X)                          |            | -0.62
        |          18  CH2 (C)(C)                       |            | -2.70
        |           1  CH2 (C)(O)                       |            | -0.13
        |           1  O-H (C)                          |            |  4.45
--------+-----------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   |  1.00
--------+-----------------------------------------------+------------+--------
HENRYs LAW CONSTANT at 25 deg C = 2.45E-003 atm-m3/mole
                                = 1.00E-001 unitless
                                = 2.48E+002 Pa-m3/mole


For Henry LC Comparison Purposes:
  Exper Database:  none available
  User-Entered Henry LC:  not entered
  Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
     HLC:  9.678E-005 atm-m3/mole  (9.806E+000 Pa-m3/mole)
     VP:   5.24E-007 mm Hg (source: MPBPVP)
     WS:   0.00213 mg/L (source: WSKOWWIN)
```

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 9.720

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
---------- KOAWIN v1.10 Results ----------

Experimental Database Structure Match:
Name : 1-Eicosanol
CAS Num : 000629-96-9
Exp LogKoa: 12.06
Exp Ref : Abraham,MH et al. (2001)

Log Koa (octanol/air) estimate: 9.720
Koa (octanol/air) estimate: 5.253e+009
Using:
Log Kow: 8.30 (user entered)
HenryLC: 0.000929 atm-m3/mole (HenryWin est)
Log Kaw: -1.420 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 8.70 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 0.000929 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 10.120 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:
==========
SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.1084	0.1084
Frag	1	Aliphatic alcohol [-OH]	0.1587	0.1587
MolWt	*	Molecular Weight Parameter		-0.1421
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.8726

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	1.8437	1.8437
Frag	1	Aliphatic alcohol [-OH]	1.1178	1.1178
MolWt	*	Molecular Weight Parameter		-4.2395

RESULT	Biowin2 (Non-Linear Biodeg Probability)		0.8495

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.2983	0.2983
Frag	1	Aliphatic alcohol [-OH]	0.1600	0.1600
MolWt	*	Molecular Weight Parameter		-0.6598
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.9977

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.2691	0.2691
Frag	1	Aliphatic alcohol [-OH]	0.1294	0.1294
MolWt	*	Molecular Weight Parameter		-0.4307
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.8155

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1611	0.1611
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	19	-CH2- [linear]	0.0494	0.9389
MolWt	*	Molecular Weight Parameter		-0.8882
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.9244

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.0041	1.0041
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	19	-CH2- [linear]	0.4295	8.1604
MolWt	*	Molecular Weight Parameter		-8.6190
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.9565

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	-0.3177	-0.3177
Frag	1	Aliphatic alcohol [-OH]	0.1328	0.1328
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Frag	19	-CH2- [linear]	0.0260	0.4938
Const	*	Equation Constant		0.8361

RESULT	Biowin7 (Anaerobic Linear Biodeg Prob)		1.0654

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

BioHCwin (v1.01) Program Results:

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

BioHCwin v1.01 Results

NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 1.47E-005 Pa (1.1E-007 mm Hg)
Log Koa (Exp database): 12.060
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.205
Octanol/air (Koa) model: 0.282
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.881
Mackay model : 0.942
Octanol/air (Koa) model: 0.958

AOP Program (v1.92) Results:

SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56

SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C)

Hydrogen Abstraction = 29.3588 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 29.4988 E-12 cm3/molecule-sec
HALF-LIFE = 0.363 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 4.351 Hrs

SUMMARY (AOP v1.91): OZONE REACTION (25 deg C)

****** NO OZONE REACTION ESTIMATION ******

(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
  0.912 (Junge-Pankow, Mackay avg)
  0.958 (Koa method)
     Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:
==============================
SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM   : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
-------------------------- KOCWIN v2.00 Results --------------------------

  Koc Estimate from MCI:

         First Order Molecular Connectivity Index .... : 10.414
         Non-Corrected Log Koc (0.5213 MCI + 0.60) .... : 6.0287
         Fragment Correction(s):
                  1   Aliphatic Alcohol (-C-OH) .... : -1.3179
         Corrected Log Koc .... : 4.7108

                          Estimated Koc: 5.138e+004 L/kg   <==========

  Koc Estimate from Log Kow:

         Log Kow (User entered   ) .... : 8.30
         Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 5.5161
         Fragment Correction(s):
                  1   Aliphatic Alcohol (-C-OH) .... : -0.4114
         Corrected Log Koc .... : 5.1046

                          Estimated Koc: 1.272e+005 L/kg   <==========

HYDROWIN Program (v2.00) Results:
================================
SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM   : 1-Eicosanol
MOL FOR: C20 H42 O1
MOL WT : 298.56
--------------------------- HYDROWIN v2.00 Results ---------------------------

 Currently, this program can NOT estimate a hydrolysis rate constant for
                the type of chemical structure entered!!

 ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
      Specific Alkyl Halides & Phosphorus Esters can be estimated!!

   When present, various hydrolyzable compound-types will be identified.
  For more information, (Click OVERVIEW in Help or see the User's Guide)

              *****   CALCULATION NOT PERFORMED   *****

BCFBAF Program (v3.01) Results:
==============================
SMILES : CCCCCCCCCCCCCCCCCCCCO
CHEM   : 1-Eicosanol

MOL FOR: C20 H42 O1
MOL WT : 298.56
---------- BCFBAF v3.01 ----------
Summary Results:
  Log BCF (regression-based estimate): 2.89 (BCF = 777 L/kg wet-wt)
  Biotransformation Half-Life (days) : 8.42 (normalized to 10 g fish)
  Log BAF (Arnot-Gobas upper trophic): 3.88 (BAF = 7.65e+003 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 8.30 (user entered)

Equation Used to Make BCF estimate:
   Log BCF = -0.49 log Kow + 7.554 + Correction

      Correction(s):   Value
       Alkyl chains (8+ -CH2- groups) -0.596

   Estimated Log BCF = 2.890 (BCF = 777.1 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.0341	0.0341
Frag	1	Aliphatic alcohol [-OH]	-0.0616	-0.0616
Frag	1	Methyl [-CH3]	0.2451	0.2451
Frag	19	-CH2- [linear]	0.0242	0.4596
L Kow	*	Log Kow = 8.30 (user-entered)	0.3073	2.5509
MolWt	*	Molecular Weight Parameter		-0.7656
Const	*	Equation Constant		-1.5371
RESULT		LOG Bio Half-Life (days)		0.9255
RESULT		Bio Half-Life (days)		8.424
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

Biotransformation Rate Constant:
 kM (Rate Constant): 0.08229 /day (10 gram fish)
 kM (Rate Constant): 0.04627 /day (100 gram fish)
 kM (Rate Constant): 0.02602 /day (1 kg fish)
 kM (Rate Constant): 0.01463 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
   Estimated Log BCF (upper trophic) = 1.904 (BCF = 80.24 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 3.884 (BAF = 7651 L/kg wet-wt)
   Estimated Log BCF (mid trophic) = 2.043 (BCF = 110.4 L/kg wet-wt)
   Estimated Log BAF (mid trophic) = 4.260 (BAF = 1.818e+004 L/kg wet-wt)
   Estimated Log BCF (lower trophic) = 2.086 (BCF = 121.8 L/kg wet-wt)
   Estimated Log BAF (lower trophic) = 4.486 (BAF = 3.06e+004 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
   Estimated Log BCF (upper trophic) = 3.369 (BCF = 2339 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 6.996 (BAF = 9.901e+006 L/kg wet-wt)

Volatilization From Water

Chemical Name: 1-Eicosanol

Molecular Weight : 298.56 g/mole
Water Solubility : -----
Vapor Pressure : -----

Henry's Law Constant: 0.000929 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	2.852	176
HALF-LIFE (days) :	0.1188	7.333

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========

(using 10000 hr Bio P,A,S)
PROPERTIES OF: 1-Eicosanol

Molecular weight (g/mol)	298.56
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	0.000929
Air-water partition coefficient	0.0379933
Octanol-water partition coefficient (Kow)	1.99526E+008
Log Kow	8.3
Biomass to water partition coefficient	3.99053E+007
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	9999.88	10000.00
-Aeration tank	0.00	9999.88	10000.00
-Settling tank	0.00	9999.88	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.3E-002	100.00
Primary sludge	5.99E+000	2.0E-002	59.89
Waste sludge	3.34E+000	1.1E-002	33.36
Primary volatilization	1.32E-005	4.4E-008	0.00
Settling volatilization	2.92E-005	9.8E-008	0.00
Aeration off gas	3.45E-004	1.2E-006	0.00
Primary biodegradation	1.75E-002	5.9E-005	0.18
Settling biodegradation	4.26E-003	1.4E-005	0.04
Aeration biodegradation	5.61E-002	1.9E-004	0.56
Final water effluent	5.97E-001	2.0E-003	5.97
Total removal	9.40E+000	3.1E-002	94.03
Total biodegradation	7.79E-002	2.6E-004	0.78

Level III Fugacity Model (Full-Output):
==========

Chem Name   : 1-Eicosanol
Molecular Wt: 298.56
Henry's LC : 0.000929 atm-m3/mole (Henrywin program)
Vapor Press : 5.24e-007 mm Hg (Mpbpwin program)
Liquid VP   : 1.27e-006 mm Hg (super-cooled)
Melting Pt : 64 deg C (user-entered)
Log Kow   : 8.3 (user-entered)
Soil Koc   : 5.14e+004 (KOCWIN MCI method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)

Air	0.678	8.7	1000
Water	21.1	360	1000
Soil	75.3	720	1000
Sediment	2.91	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.98e-012	828	104	27.6	3.46
Water	4.55e-010	622	323	20.7	10.8
Soil	1.62e-010	1.11e+003	0	37.1	0
Sediment	2.81e-010	9.54	0.892	0.318	0.0297

Persistence Time: 511 hr
Reaction Time: 596 hr
Advection Time: 3.58e+003 hr
Percent Reacted: 85.7
Percent Advected: 14.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 8.702
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 2.998 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004