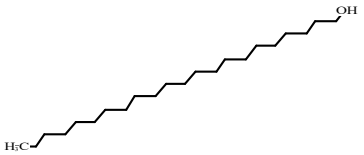
CAS Number: 661-19-8
SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61

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

Physical Property Inputs:

Log Kow (octanol-water):	8.40
Boiling Point (deg C) :	------
Melting Point (deg C) :	71.00
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 : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	21	-CH2- [aliphatic carbon]	0.4911	10.3131
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Const		Equation Constant		0.2290
			Log Kow =	9.6808

MPBPVP (v1.43) Program Results:

Experimental Database Structure Match:

Name :	1-Docosanol
CAS Num :	000661-19-8
Exp MP (deg C):	72.5
Exp BP (deg C):	180 @ 0.22 mm Hg
Exp VP (mm Hg):	---

SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61

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

Boiling Point: 401.08 deg C (Adapted Stein and Brown Method)

Melting Point: 125.36 deg C (Adapted Joback Method)
Melting Point: 120.53 deg C (Gold and Ogle Method)
Mean Melt Pt : 122.94 deg C (Joback; Gold,Ogle Methods)
Selected MP: 122.94 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 401.08 deg C (estimated))
(Using MP: 71.00 deg C (user entered))
VP: 9.51E-009 mm Hg (Antoine Method)
: 1.27E-006 Pa (Antoine Method)
VP: 6.34E-008 mm Hg (Modified Grain Method)
: 8.45E-006 Pa (Modified Grain Method)
VP: 5.65E-006 mm Hg (Mackay Method)
: 0.000753 Pa (Mackay Method)
Selected VP: 6.34E-008 mm Hg (Modified Grain Method)

: 8.45E-006 Pa (Modified Grain Method)
Subcooled liquid VP: 1.72E-007 mm Hg (25 deg C, Mod-Grain method)
: 2.29E-005 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	21	-CH2-	24.22	508.62
Group	1	-OH (primary)	88.46	88.46
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		817.24
RESULT- corr		BOILING POINT in deg Kelvin		674.24
		BOILING POINT in deg C		401.08

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	21	-CH2-	11.27	236.67
Group	1	-OH (primary)	44.45	44.45
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		398.52
		MELTING POINT in deg C		125.36

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

Water Sol: 0.001313 mg/L

SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
---------- WSKOW v1.42 Results ----------
Log Kow (estimated) : 9.68
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 8.40 (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) = 71.00 deg C (Use Tm = 25 for all liquids)

Correction(s):	Value
Alcohol, aliphatic	0.424

Log Water Solubility (in moles/L) : -8.396
Water Solubility at 25 deg C (mg/L): 0.001313

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

Water Sol (v1.01 est): 5.832e-005 mg/L

SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	21	-CH2- [aliphatic carbon]	-0.5370	-11.2774
Frag	1	-OH [hydroxy, aliphatic attach]	1.6012	1.6012
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -9.7482
Water Solubility (mg/L) at 25 dec C =5.832e-005

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

SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
CAS Num:
ChemID1:
MOL FOR: C22 H46 O1
MOL WT : 326.61
Log Kow: 9.681 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: 71.00 (deg C, User Entered for Wat Sol estimate)
Melt Pt: 72.50 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 7.739E-005 (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: 9.681 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 7.739E-005 (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	3.39e-005
Neutral Organics	Daphnid	48-hr	LC50	3.91e-005
Neutral Organics	Green Algae	96-hr	EC50	0.000547 *
Neutral Organics	Fish		ChV	7.65e-006
Neutral Organics	Daphnid		ChV	2.75e-005
Neutral Organics	Green Algae		ChV	0.000695 *
Neutral Organics	Fish (SW)	96-hr	LC50	4.47e-005
Neutral Organics	Mysid	96-hr	LC50	1.83e-007
Neutral Organics	Fish (SW)		ChV	0.000528 *
Neutral Organics	Mysid (SW)		ChV	1.62e-009
Neutral Organics	Earthworm	14-day	LC50	90.726 *

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 :  1.64E-003 atm-m3/mole  (1.66E+002 Pa-m3/mole)
       Group Est:  4.88E-003 atm-m3/mole  (4.95E+002 Pa-m3/mole)

SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM   : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
--------------------------- HENRYWIN v3.20 Results -------------------------
----------+-----------------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION             | COMMENT |  VALUE
----------+-----------------------------------------------+---------+----------
 HYDROGEN |  45  Hydrogen to Carbon (aliphatic) Bonds     |         | -5.3855
 HYDROGEN |   1  Hydrogen to Oxygen Bonds                 |         |  3.2318
 FRAGMENT |  21  C-C                                      |         |  2.4424
 FRAGMENT |   1  C-O                                      |         |  1.0855
 FACTOR   |   *  Non-cyclic alkyl or olefinic alcohol     |         |  -.2000
----------+-----------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE     |  TOTAL  |  1.174
----------+-----------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 1.64E-003 atm-m3/mole
                                = 6.70E-002 unitless
                                = 1.66E+002 Pa-m3/mole

--------+-----------------------------------------------+------------+--------
        |        GROUP CONTRIBUTION DESCRIPTION         |   COMMENT  |  VALUE
--------+-----------------------------------------------+------------+--------
        |           1  CH3 (X)                          |            | -0.62
        |          20  CH2 (C)(C)                       |            | -3.00
        |           1  CH2 (C)(O)                       |            | -0.13
        |           1  O-H (C)                          |            |  4.45
--------+-----------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   |  0.70
--------+-----------------------------------------------+------------+--------
HENRYs LAW CONSTANT at 25 deg C = 4.88E-003 atm-m3/mole
                                = 2.00E-001 unitless
                                = 4.95E+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:  2.075E-005 atm-m3/mole  (2.103E+000 Pa-m3/mole)
     VP:   6.34E-008 mm Hg (source: MPBPVP)
     WS:   0.00131 mg/L (source: WSKOWWIN)


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

Log Koa: 9.574

SMILES : CCCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 9.574
Koa (octanol/air) estimate: 3.746e+009
Using:
Log Kow: 8.40 (user entered)
HenryLC: 0.00164 atm-m3/mole (HenryWin est)
Log Kaw: -1.174 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 9.68 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 0.00164 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 10.854 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:
==========
SMILES : CCCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
---------- 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		-0.1555
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.8592

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		-4.6379
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.7912

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		-0.7218
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.9357

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		-0.4712
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.7750

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	21	-CH2- [linear]	0.0494	1.0377
MolWt	*	Molecular Weight Parameter		-0.9717
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.9398

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	21	-CH2- [linear]	0.4295	9.0194
MolWt	*	Molecular Weight Parameter		-9.4289
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.9585

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	21	-CH2- [linear]	0.0260	0.5458
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		1.1173

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 : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
---------- 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): 2.29E-005 Pa (1.72E-007 mm Hg)
Log Koa (Koawin est): 9.574
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.131
Octanol/air (Koa) model: 0.00092
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.825
Mackay model : 0.913
Octanol/air (Koa) model: 0.0686

AOP Program (v1.92) Results:
==========
SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 32.1849 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 = 32.3249 E-12 cm3/molecule-sec
HALF-LIFE = 0.331 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 3.971 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):
0.869 (Junge-Pankow, Mackay avg)
0.0686 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

```
KOCWIN Program (v2.00) Results:
==============================
SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM   : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
--------------------------  KOCWIN v2.00 Results  --------------------------

  Koc Estimate from MCI:
  ----------------------
         First Order Molecular Connectivity Index  ..........  : 11.414
         Non-Corrected Log Koc (0.5213 MCI + 0.60)  ..........  :  6.5500
         Fragment Correction(s):
                  1   Aliphatic Alcohol  (-C-OH)  ..........  : -1.3179
         Corrected Log Koc  ..................................  :  5.2321

                         Estimated Koc:  1.707e+005  L/kg   <==========

  Koc Estimate from Log Kow:
  --------------------------
         Log Kow  (User entered   )  ........................  :  8.40
         Non-Corrected Log Koc (0.55313 logKow + 0.9251)  ....  :  5.5714
         Fragment Correction(s):
                  1   Aliphatic Alcohol  (-C-OH)  ..........  : -0.4114
         Corrected Log Koc  ..................................  :  5.1599

                         Estimated Koc:  1.445e+005  L/kg   <==========



HYDROWIN Program (v2.00) Results:
=================================
SMILES : CCCCCCCCCCCCCCCCCCCCCCO
CHEM   : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
--------------------------- 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 : CCCCCCCCCCCCCCCCCCCCCCO
CHEM   : Docosan-1-ol
MOL FOR: C22 H46 O1
MOL WT : 326.61
-------------------------------- BCFBAF v3.01 --------------------------------
Summary Results:
  Log BCF (regression-based estimate):  2.84  (BCF = 694 L/kg wet-wt)
  Biotransformation Half-Life (days) :  8.56  (normalized to 10 g fish)
  Log BAF (Arnot-Gobas upper trophic):  3.82  (BAF = 6.62e+003 L/kg wet-wt)

Log Kow (experimental):  not available from database
```

Log Kow used by BCF estimates: 8.40 (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 = 2.842 (BCF = 694.2 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	21	-CH2- [linear]	0.0242	0.5079
L Kow	*	Log Kow = 8.40 (user-entered)	0.3073	2.5817
MolWt	*	Molecular Weight Parameter		-0.8375
Const	*	Equation Constant		-1.5371
RESULT		LOG Bio Half-Life (days)		0.9327
RESULT		Bio Half-Life (days)		8.564
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

Biotransformation Rate Constant:
 kM (Rate Constant): 0.08094 /day (10 gram fish)
 kM (Rate Constant): 0.04552 /day (100 gram fish)
 kM (Rate Constant): 0.0256 /day (1 kg fish)
 kM (Rate Constant): 0.01439 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
   Estimated Log BCF (upper trophic) = 1.816 (BCF = 65.41 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 3.821 (BAF = 6621 L/kg wet-wt)
   Estimated Log BCF (mid trophic)   = 1.954 (BCF = 89.94 L/kg wet-wt)
   Estimated Log BAF (mid trophic)   = 4.191 (BAF = 1.552e+004 L/kg wet-wt)
   Estimated Log BCF (lower trophic) = 1.996 (BCF = 99.19 L/kg wet-wt)
   Estimated Log BAF (lower trophic) = 4.414 (BAF = 2.591e+004 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
   Estimated Log BCF (upper trophic) = 3.306 (BCF = 2025 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 6.948 (BAF = 8.876e+006 L/kg wet-wt)

Volatilization From Water

Chemical Name: Docosan-1-ol

Molecular Weight   : 326.61 g/mole
Water Solubility   : -----
Vapor Pressure   : -----
Henry's Law Constant: 0.00164 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) :	2.489	178.7

HALF-LIFE (days) : 0.1037 7.446

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

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

Molecular weight (g/mol)	326.61
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	0.00164
Air-water partition coefficient	0.0670711
Octanol-water partition coefficient (Kow)	2.51188E+008
Log Kow	8.4
Biomass to water partition coefficient	5.02377E+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	9999.90	10000.00
-Aeration tank	0.00	9999.90	10000.00
-Settling tank	0.00	9999.90	10000.00

STP Overall Chemical Mass Balance:
---

	g/h	mol/h	percent
Influent	1.00E+001	3.1E-002	100.00
Primary sludge	5.99E+000	1.8E-002	59.89
Waste sludge	3.34E+000	1.0E-002	33.36
Primary volatilization	1.15E-005	3.5E-008	0.00
Settling volatilization	2.55E-005	7.8E-008	0.00
Aeration off gas	4.84E-004	1.5E-006	0.00
Primary biodegradation	1.75E-002	5.4E-005	0.18
Settling biodegradation	4.26E-003	1.3E-005	0.04
Aeration biodegradation	5.61E-002	1.7E-004	0.56
Final water effluent	5.97E-001	1.8E-003	5.97
Total removal	9.40E+000	2.9E-002	94.03
Total biodegradation	7.79E-002	2.4E-004	0.78

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

Chem Name : Docosan-1-ol
Molecular Wt: 326.61
Henry's LC : 0.00164 atm-m3/mole (Henrywin program)
Vapor Press : 6.34e-008 mm Hg (Mpbpwin program)
Liquid VP : 1.81e-007 mm Hg (super-cooled)
Melting Pt : 71 deg C (user-entered)
Log Kow : 8.4 (user-entered)
Soil Koc : 1.71e+005 (KOCWIN MCI method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.51	7.94	1000
Water	19.1	360	1000
Soil	73.4	720	1000
Sediment	6.99	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.08e-012	751	86.1	25	2.87
Water	5.86e-010	621	323	20.7	10.8

Soil	8.43e-011	1.19e+003	0	39.7	0
Sediment	3.61e-010	25.2	2.36	0.841	0.0786

Persistence Time: 562 hr
Reaction Time: 652 hr
Advection Time: 4.1e+003 hr
Percent Reacted: 86.3
Percent Advected: 13.7

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 7.942
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 2.936 (weeks)

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