United States
Environmental Protection Agency

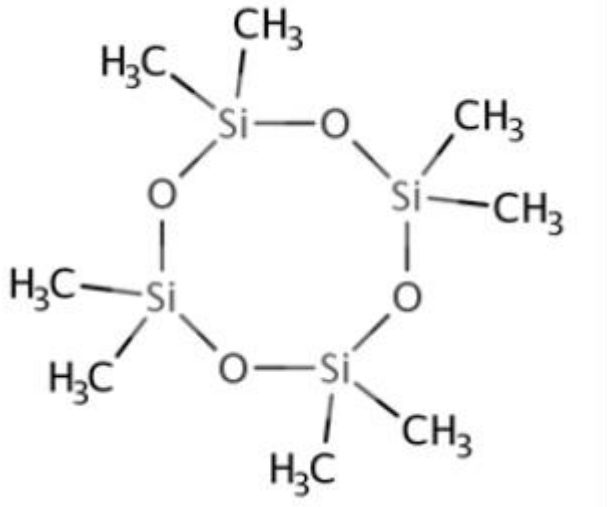
September 2025
Office of Chemical Safety and
Pollution Prevention

Draft Risk Evaluation for Octamethylcyclotetrasiloxane (D4)

Supplemental Information File:

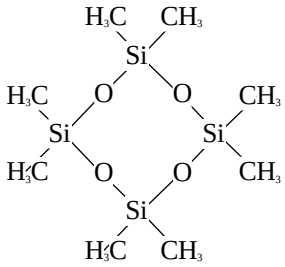
Physical Chemistry and Fate Assessment EPI Suite Model Outputs for Octamethylcyclotetrasiloxane (D4)

CASRN 556-67-2



September 2025

EPI Suite Results For CAS 556-67-2



SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): 6.49
Boiling Point (deg C) : 175.00
Melting Point (deg C) : 17.50
Vapor Pressure (mm Hg) : 0.9338
Water Solubility (mg/L): 0.056
Henry LC (atm-m3/mole) : 11.8

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

Log Kow(version 1.68 estimate): 6.79

Experimental Database Structure Match:
Name : OCTAMETHYLTETRASILOXANE
CAS Num : 000556-67-2
Exp Log P: 6.74
Exp Ref : SEHSC (2009); average

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	-CH3 [aliphatic carbon]	0.5473	4.3784
Frag	4	-Si- [silicon, aromatic or oxygen attach]	0.6800	2.7200
Frag	4	-O- [oxygen, two silicon attach, cyclic]	-0.1348	-0.5392
Factor	4	Cyclic Si-O-Si correction [coef * NUM - 4]	-0.4948	0.0000
Const		Equation Constant		0.2290

Log Kow = 6.7882

```
MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
Name     :  OCTAMETHYLTETRASILOXANE
CAS Num  :  000556-67-2
Exp MP (deg C):  17.5
Exp BP (deg C):  175.8
Exp VP (mm Hg):  1.05E+00  (extrapolated)
       (Pa   ):  1.40E+002
Exp VP (deg C):  25
Exp VP ref    :  FLANINGAM,OL (1986)

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
----------------------- SUMMARY MPBVP v1.43 --------------------

Boiling Point:  159.41 deg C (Adapted Stein and Brown Method)
Melting Point:   24.14 deg C (Adapted Joback Method)
Melting Point:  -20.58 deg C (Gold and Ogle Method)
Mean Melt Pt :    1.78 deg C (Joback; Gold,Ogle Methods)
Selected MP:    1.78 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 175.00 deg C (user entered))
(MP not used for liquids)
VP:  1.34 mm Hg (Antoine Method)
  :  179 Pa  (Antoine Method)
VP:  1.12 mm Hg (Modified Grain Method)
  :  149 Pa  (Modified Grain Method)
VP:  1.72 mm Hg (Mackay Method)
  :  229 Pa  (Mackay Method)
Selected VP:  1.23 mm Hg (Mean of Antoine & Grain methods)
  :  164 Pa  (Mean of Antoine & Grain methods)

-------+-----+--------------------+----------+---------
TYPE   | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  8  |  -CH3              |   21.98  |  175.84
Group |  4  |  -O-   (ring)      |   32.98  |  131.92
Group |  4  |  Si (ring)         | regress  |  -75.86
*     |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  430.08
RESULT- corr |  BOILING POINT in deg Kelvin  |  432.57
|  BOILING POINT in deg C       |  159.41
-------------------------------------------------------

-------+-----+--------------------+----------+---------
TYPE   | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  8  |  -CH3              |   -5.10  |  -40.80
Group |  4  |  -O-   (ring)      |   23.05  |   92.20
Group |  4  |  Si (ring)         | regress  |  123.40
*     |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
```

```
RESULT    |  MELTING POINT in deg Kelvin  |  297.30
          |  MELTING POINT in deg C       |   24.14
-----------------------------------------------------


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

Water Sol: 0.1083 mg/L

Experimental Water Solubility Database Match:
Name     :  OCTAMETHYLTETRASILOXANE
CAS Num  :  000556-67-2
Exp WSol :  0.005 mg/L (25 deg C)
Exp Ref  :  DOW CORNING (1987)

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
---------------------------------- WSKOW v1.42 Results -----------------------
Log Kow  (estimated)  :  6.79
Log Kow (experimental):  6.74
Cas No: 000556-67-2
Name  : OCTAMETHYLTETRASILOXANE
Refer : SEHSC (2009); average
Log Kow used by Water solubility estimates:  6.49 (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) = 17.50 deg C (Use Tm = 25 for all liquids)

Correction(s):         Value
--------------------   -----
Cyclic Siloxane       0.029  [4 Si-O-Si unit(s)]

Log Water Solubility  (in moles/L) :  -6.438
Water Solubility at 25 deg C (mg/L):  0.1083



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

Water Sol (v1.01 est): 0.17229 mg/L

Experimental Water Solubility Database Match:
Name     :  OCTAMETHYLTETRASILOXANE
CAS Num  :  000556-67-2
Exp WSol :  0.005 mg/L (25 deg C)
Exp Ref  :  DOW CORNING (1987)

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
```

```
-------+-----+-------------------------------------------+----------+---------
TYPE   | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION   |  COEFF   |  VALUE
-------+-----+-------------------------------------------+----------+---------
Frag   |  8  |  -CH3    [aliphatic carbon]                |-0.3213   | -2.5702
Frag   |  4  |  -Si-  [silicon, aromatic or oxygen attach]| 0.0000   |  0.0000
Frag   |  4  |  -O-  [oxygen, two silicon attach, cyclic] |-2.7000   | -3.9150
Const  |     |  Equation Constant                        |          |  0.2492
-------+-----+-------------------------------------------+----------+---------
Log Water Sol (moles/L) at 25 dec C  =   -6.2360
Water Solubility (mg/L) at 25 dec C  =  0.17229


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

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
CAS Num:
ChemID1:
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
Log Kow: 6.788      (EPISuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow: 6.74       (PhysProp DB exp value - for comparison only)
Melt Pt: 17.50      (deg C, User Entered for Wat Sol estimate)
Melt Pt: 17.50      (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.06203    (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 0.056      (mg/L, User Entered)
Wat Sol: 0.005      (mg/L, PhysProp DB exp value)

-------------------------------------
Values used to Generate ECOSAR Profile
-------------------------------------
Log Kow: 6.788      (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 0.056      (mg/L, User Entered)

-------------------------------------
ECOSAR v1.11 Class-specific Estimations
-------------------------------------
Neutral Organics
Predicted
ECOSAR Class                  Organism            Duration  End Pt   mg/L (ppm)
============================  ==================  ========  ======   ==========
Neutral Organics           : Fish                96-hr     LC50        0.012
Neutral Organics           : Daphnid             48-hr     LC50        0.011
Neutral Organics           : Green Algae         96-hr     EC50        0.050
Neutral Organics           : Fish                          ChV         0.002
Neutral Organics           : Daphnid                       ChV         0.004
Neutral Organics           : Green Algae                   ChV         0.035
Neutral Organics           : Fish (SW)           96-hr     LC50        0.016
Neutral Organics           : Mysid               96-hr     LC50     0.000459
Neutral Organics           : Fish (SW)                     ChV         0.032
Neutral Organics           : Mysid (SW)                    ChV     9.59e-006
Neutral Organics           : Earthworm           14-day    LC50      164.386 *
```

```
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 :  8.72E-002 atm-m3/mole  (8.84E+003 Pa-m3/mole)
Group Est:  Incomplete

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
--------------------------- HENRYWIN v3.20 Results -------------------------

Experimental Database Structure Match:
Name     :  OCTAMETHYLTETRASILOXANE
CAS Num  :  000556-67-2
Exp HLC  :  1.17E-01 atm-m3/mole  (1.19E+004 Pa-m3/mole)
Temper   :  25 deg C
Exp Ref  :  HAMELINK,JL ET AL. (1996)

----------+-----------------------------------------------+---------+----------
CLASS  |     BOND CONTRIBUTION DESCRIPTION           | COMMENT |  VALUE
----------+-----------------------------------------------+---------+----------
HYDROGEN |  24  Hydrogen to Carbon (aliphatic) Bonds   |         | -2.8722
FRAGMENT |   8  C-Si                                   | ESTIMATE|  0.9600
FRAGMENT |   8  O-Si                                   | ESTIMATE|  1.3600
----------+-----------------------------------------------+---------+----------
RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE   |  TOTAL  | -0.552
----------+-----------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 8.72E-002 atm-m3/mole
= 3.57E+000 unitless
= 8.84E+003 Pa-m3/mole

--------+-----------------------------------------------+------------+--------
|        GROUP CONTRIBUTION DESCRIPTION         |   COMMENT  |  VALUE
--------+-----------------------------------------------+------------+--------
|              MISSING Value for:  CH3 (Si)
|              MISSING Value for:  UNTYPED(O)(C)(O)(C)
|              MISSING Value for:  CH3 (Si)
|              MISSING Value for:  O (Si)(Si)
```

```
|              MISSING Value for:  UNTYPED(C)(C)(O)(O)
|              MISSING Value for:  CH3 (Si)
|              MISSING Value for:  CH3 (Si)
|              MISSING Value for:  O (Si)(Si)
|              MISSING Value for:  UNTYPED(C)(C)(O)(O)
|              MISSING Value for:  CH3 (Si)
--------+-------------------------------------------------+------------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |  0.00
--------+-------------------------------------------------+------------+--------

For Henry LC Comparison Purposes:
Exper Database: 1.17E-01  atm-m3/mole  (1.19E+004 Pa-m3/mole)
User-Entered Henry LC:  1.180E+001 atm-m3/mole  (1.196E+006 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  6.508E+000 atm-m3/mole  (6.594E+005 Pa-m3/mole)
VP:   0.934 mm Hg (source: User-Entered)
WS:   0.056 mg/L (source: User-Entered)


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

Log Koa: 3.805

SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
--------------------------- KOAWIN v1.10 Results --------------------------

Log Koa (octanol/air) estimate:  3.805
Koa (octanol/air) estimate:  6376
Using:
Log Kow:  6.49  (user entered)
HenryLC:  11.8  atm-m3/mole (user entered)
Log Kaw:  2.683  (air/water part.coef.)

LogKow  : 6.74 (exp database)
LogKow  : 6.79 (KowWin estimate)
Henry LC: 0.117 atm-m3/mole (exp database)
Henry LC: 0.0872 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate:  6.238 (from KowWin/HenryWin)


BIOWIN (v4.10) Program Results:
===============================
SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
--------------------------- BIOWIN v4.10 Results ---------------------------

Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
```

```
Biowin5 (MITI Linear Model Prediction)    :  Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction):  Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter               |         | -0.1412
Const|  *  |  Equation Constant                        |         |  0.7475
============+=========================================+=========+=========
RESULT   |    Biowin1 (Linear Biodeg Probability)     |         |  0.6063
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter               |         | -4.2120
============+=========================================+=========+=========
RESULT   |  Biowin2 (Non-Linear Biodeg Probability)   |         |  0.2309
============+=========================================+=========+=========

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
------+-----+-----------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter               |         | -0.6555
Const|  *  |  Equation Constant                        |         |  3.1992
============+=========================================+=========+=========
RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)  |         |  2.5437
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter               |         | -0.4280
Const|  *  |  Equation Constant                        |         |  3.8477
============+=========================================+=========+=========
RESULT   |   Biowin4 (Survey Model - Primary Biodeg)  |         |  3.4198
============+=========================================+=========+=========

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 |  8  |  Methyl  [-CH3]                           |  0.0004 |  0.0033
MolWt|  *  |  Molecular Weight Parameter               |         | -0.8824
Const|  *  |  Equation Constant                        |         |  0.7121
============+=========================================+=========+=========
RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         | -0.1670
============+=========================================+=========+=========
```

```
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  8  |  Methyl  [-CH3]                          |  0.0194 |  0.1554
MolWt|  *  |  Molecular Weight Parameter              |         | -8.5631
============+=========================================+=========+=========
RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.0028
============+=========================================+=========+=========

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 |  8  |  Methyl  [-CH3]                          | -0.0796 | -0.6366
Const|  *  |  Equation Constant                       |         |  0.8361
============+=========================================+=========+=========
RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |         |  0.1995
============+=========================================+=========+=========

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 : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
-------------------------- 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):  125 Pa (0.934 mm Hg)
Log Koa (Koawin est  ): 3.805
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  2.41E-008
Octanol/air (Koa) model:  1.57E-009
Fraction sorbed to airborne particulates (phi):
```

```
Junge-Pankow model     :  8.7E-007
Mackay model           :  1.93E-006
Octanol/air (Koa) model:  1.25E-007


AOP Program (v1.92) Results:
============================
SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction       =   1.1968 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 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 =   1.1968 E-12 cm3/molecule-sec
HALF-LIFE =     8.937 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE =   107.246 Hrs
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------

******  NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:
Chem Name :  Octamethylcyclotetrasiloxane
CAS Number:  000556-67-2
Exper OH rate constant   :  1.01  E-12  cm3/molecule-sec
Exper OH Reference:  ATKINSON,R (1991)
Exper Ozone rate constant:  < 3 E-20  cm3/molecule-sec
Exper NO3 rate constant  :  < 1.4 E-16  cm3/molecule-sec
Fraction sorbed to airborne particulates (phi):
1.4E-006 (Junge-Pankow, Mackay avg)
1.25E-007 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation


KOCWIN Program (v2.00) Results:
===============================
SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
---------------------------  KOCWIN v2.00 Results  --------------------------

Koc Estimate from MCI:
----------------------
First Order Molecular Connectivity Index  ..........  :  6.828
Non-Corrected Log Koc (0.5213 MCI + 0.60)  ..........  :  4.1595
Fragment Correction(s) -->  NONE                       :   ---
Corrected Log Koc  ................................... :  4.1595

Estimated Koc:  1.444e+004  L/kg   <===========
```

```
Koc Estimate from Log Kow:
--------------------------
Log Kow  (User entered   )  ......................... :  6.49
Non-Corrected Log Koc (0.8679 logKow - 0.0004)  ..... :  5.6305
Fragment Correction(s) -->  NONE                      :   ---
Corrected Log Koc  ................................. :  5.6305

Estimated Koc:  4.271e+005  L/kg   <===========


HYDROWIN Program (v2.00) Results:
=================================
SMILES : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
--------------------------- 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 : C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
CHEM   : Cyclotetrasiloxane, octamethyl-
MOL FOR: C8 H24 O4 Si4
MOL WT : 296.62
--------------------------------- BCFBAF v3.01 ---------------------------------
Summary Results:
Log BCF (regression-based estimate):  3.95  (BCF = 8.87e+003 L/kg wet-wt)
Biotransformation Half-Life (days) :  45.4  (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic):  6.12  (BAF = 1.32e+006 L/kg wet-wt)

Experimental BCF-kM Database Structure Match:
---------------------------------------------
Name      :  Cyclotetrasiloxane, octamethyl-
CAS Num   :  000556-67-2
Log BCF   :  ---
BCF Data  :  ---
Log Bio HL:  1.881  (Bio Half-life = 76 days)
Bio Data  :  kM Training Set

Log Kow (experimental):  6.74
Log Kow used by BCF estimates:  6.49 (user entered)

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction
```

```
Correction(s):                    Value
No Applicable Correction Factors

Estimated Log BCF =  3.948  (BCF = 8867 L/kg wet-wt)

============================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
============================================================
------+-----+-------------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
Frag |  8  |  Methyl  [-CH3]                           |  0.2451 |  1.9608
L Kow|  *  |  Log Kow =   6.49 (user-entered   )       |  0.3073 |  1.9940
MolWt|  *  |  Molecular Weight Parameter               |         | -0.7606
Const|  *  |  Equation Constant                        |         | -1.5371
============+===========================================+=========+=========
RESULT   |        LOG Bio Half-Life (days)            |         |  1.6572
RESULT   |            Bio Half-Life (days)            |         |   45.41
NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C   |
============+===========================================+=========+=========

Biotransformation Rate Constant:
kM (Rate Constant):  0.01526 /day (10 gram fish)
kM (Rate Constant):  0.008583 /day (100 gram fish)
kM (Rate Constant):  0.004827 /day (1 kg fish)
kM (Rate Constant):  0.002714 /day (10 kg fish)

Note: For Arnot-Gobas BCF & BAF Methods, Experimental Km Half-Life Used:
Exp Km Half-Life = 1.881 days (Rate Constant = 0.009116/ day)
Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) =  3.982  (BCF = 9592 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  6.122  (BAF = 1.324e+006 L/kg wet-wt)
Estimated Log BCF (mid trophic)   =  4.131  (BCF = 1.351e+004 L/kg wet-wt)
Estimated Log BAF (mid trophic)   =  5.920  (BAF = 8.327e+005 L/kg wet-wt)
Estimated Log BCF (lower trophic) =  4.171  (BCF = 1.481e+004 L/kg wet-wt)
Estimated Log BAF (lower trophic) =  5.776  (BAF = 5.976e+005 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) =  4.274  (BCF = 1.879e+004 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  6.835  (BAF = 6.84e+006 L/kg wet-wt)


Volatilization From Water
=========================

Chemical Name: Cyclotetrasiloxane, octamethyl-

Molecular Weight    :  296.62 g/mole
Water Solubility    :  0.056 ppm
Vapor Pressure      :  0.9338 mm Hg
Henry's Law Constant:  11.8 atm-m3/mole  (entered by user)

RIVER             LAKE
---------         ---------
Water Depth     (meters):   1                1
Wind Velocity    (m/sec):   5                0.5
```

```
Current Velocity (m/sec):   1                 0.05

HALF-LIFE (hours) :   1.758             163.6
HALF-LIFE (days ) :   0.07323           6.816


STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
==========================================================================
(using 10000 hr Bio P,A,S)
PROPERTIES OF: Cyclotetrasiloxane, octamethyl-
-------------
Molecular weight (g/mol)                                296.62
Aqueous solubility (mg/l)                               0.056
Vapour pressure (Pa)                                    124.496
(atm)                                  0.00122868
(mm Hg)                                0.9338
Henry 's law constant (Atm-m3/mol)                      11.8
Air-water partition coefficient                         482.585
Octanol-water partition coefficient (Kow)               3.0761E+006
Log Kow                                                 6.488
Biomass to water partition coefficient                  615220
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      9991.88       10000.00
-Aeration tank       0.00      9991.88       10000.00
-Settling tank       0.00      9991.88       10000.00

STP Overall Chemical Mass Balance:
----------------------------------
                               g/h              mol/h         percent

Influent                    1.00E+001         3.4E-002        100.00

Primary sludge              5.94E+000         2.0E-002         59.41
Waste sludge                4.67E-002         1.6E-004          0.47
Primary volatilization      1.07E-003         3.6E-006          0.01
Settling volatilization     3.35E-005         1.1E-007          0.00
Aeration off gas            3.98E+000         1.3E-002         39.84

Primary biodegradation      1.74E-002         5.9E-005          0.17
Settling biodegradation     5.97E-005         2.0E-007          0.00
Aeration biodegradation     7.86E-004         2.7E-006          0.01

Final water effluent        9.26E-003         3.1E-005          0.09

Total removal               9.99E+000         3.4E-002         99.91
Total biodegradation        1.82E-002         6.2E-005          0.18
(** Total removal recommended maximum is 95 percent)


Level III Fugacity Model (Full-Output):
=======================================
Chem Name    : Cyclotetrasiloxane, octamethyl-
Molecular Wt: 296.62
Henry's LC   : 11.8 atm-m3/mole (user-entered)
Vapor Press : 0.934 mm Hg  (user-entered)
Log Kow      : 6.49  (user-entered)
```

```
Soil Koc    : 1.44e+004  (KOCWIN MCI method)

Mass Amount    Half-Life    Emissions
(percent)        (hr)       (kg/hr)
Air       51.9            274          1000
Water     29.6            99.6         1000
Soil      2.65            126          1000
Sediment  15.9            5.25e+003    0

Fugacity    Reaction    Advection   Reaction    Advection
(atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       1.42e-010    437         1.72e+003   14.6        57.5
Water     1.66e-005    684         98.4        22.8        3.28
Soil      4.39e-008    48.4        0           1.61        0
Sediment  1.51e-005    6.99        1.06        0.233       0.0353

Persistence Time: 111 hr
Reaction Time:    283 hr
Advection Time:   182 hr
Percent Reacted:  39.2
Percent Advected: 60.8

Half-Lives (hr), (based upon user-entry):
Air:      273.6
Water:    99.6
Soil:     126
Sediment: 5248

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