SMILES : C(C1C(C(C(C(O1)O)O)O)O)O

CHEM :

MOL FOR: C6 H12 O6

MOL WT : 180.16

------------------------------ EPI SUMMARY (v3.20) --------------------------

Physical Property Inputs:

Water Solubility (mg/L): ------

Vapor Pressure (mm Hg) : ------

Henry LC (atm-m3/mole) : ------

Log Kow (octanol-water): ------

Boiling Point (deg C) : ------

Melting Point (deg C) : ------

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.68 estimate) = -2.89

Log Kow (Exper. database match) = -3.24

Exper. Ref: SANGSTER (1994)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.43):

Boiling Pt (deg C): 380.68 (Adapted Stein & Brown method)

Melting Pt (deg C): 132.79 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 1.33E-007 (Modified Grain method)

VP (Pa, 25 deg C) : 1.78E-005 (Modified Grain method)

MP (exp database): < 25 deg C

VP (exp database): 8.02E-14 mm Hg (**1.07E-011 Pa**) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 deg C (mg/L): 1e+006

log Kow used: -3.24 (expkow database)

no-melting pt equation used

Water Sol (Exper. database match) = 1.2e+006 mg/L (30 deg C)

Exper. Ref: MULLIN,JW (1972)

Water Sol (Exper. database match) = 5e+005 mg/L (20 deg C)

Exper. Ref: YALKOWSKY,SH & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:

Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 9.72E-015 atm-m3/mole (9.85E-010 Pa-m3/mole)

Group Method: 1.62E-026 atm-m3/mole (1.64E-021 Pa-m3/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 3.153E-014 atm-m3/mole (3.195E-009 Pa-m3/mole)

VP: 1.33E-007 mm Hg (source: MPBPVP)

WS: 1E+006 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: -3.24 (exp database)

Log Kaw used: -12.401 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 9.161

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 1.1081

Biowin2 (Non-Linear Model) : 0.9315

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 3.5922 (days-weeks )

Biowin4 (Primary Survey Model) : 4.2253 (days )

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 1.0950

Biowin6 (MITI Non-Linear Model): 0.8829

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 1.4659

Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 1.07E-011 Pa (8.02E-014 mm Hg)

Log Koa (Koawin est ): 9.161

Kp (particle/gas partition coef. (m3/ug)):

Mackay model : 2.81E+005

Octanol/air (Koa) model: 0.000356

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 1

Mackay model : 1

Octanol/air (Koa) model: 0.0277

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 104.3877 E-12 cm3/molecule-sec

Half-Life = 0.102 Days (12-hr day; 1.5E6 OH/cm3)

Half-Life = 1.230 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

1 (Junge-Pankow, Mackay avg)

0.0277 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 10 L/kg (MCI method)

Log Koc: 1.000 (MCI method)

Koc : 0.01658 L/kg (Kow method)

Log Koc: -1.781 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)

Log Biotransformation Half-life (HL) = -3.2387 days (HL = 0.0005772 days)

Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)

Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)

log Kow used: -3.24 (expkow database)

Volatilization from Water:

Henry LC: 9.72E-015 atm-m3/mole (estimated by Bond SAR Method)

Half-Life from Model River: 8.085E+010 hours (3.369E+009 days)

Half-Life from Model Lake : 8.82E+011 hours (3.675E+010 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.75 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent) (hr) (kg/hr)

Air 5.06e-007 2.46 1000

Water 28.1 208 1000

Soil 71.8 416 1000

Sediment 0.0592 1.87e+003 0

Persistence Time: 414 hr