

SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43

----- 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 v1.67 estimate) = 1.42

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.42):

Boiling Pt (deg C): 623.78 (Adapted Stein & Brown method)
Melting Pt (deg C): 270.42 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 3.52E-014 (Modified Grain method)
Subcooled liquid VP: 1.76E-011 mm Hg (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 486.5
log Kow used: 1.42 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 0.025124 mg/L

ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:
Surfactants-anionic

Henry's Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 2.86E-009 atm-m3/mole
Group Method: Incomplete
Henry's LC [VP/WSol estimate using EPI values]: 3.165E-017 atm-m3/mole

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

Log Kow used: 1.42 (KowWin est)
Log Kaw used: -6.932 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 8.352
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.3504
Biowin2 (Non-Linear Model) : 0.0357
Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.7542 (weeks)
Biowin4 (Primary Survey Model) : 3.6274 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.3674
Biowin6 (MITI Non-Linear Model): 0.1714
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5194
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 2.35E-009 Pa (1.76E-011 mm Hg)
Log Koa (Koawin est): 8.352
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 1.28E+003
Octanol/air (Koa) model: 5.52E-005
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 1
Mackay model : 1
Octanol/air (Koa) model: 0.0044

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

Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 31.4611 E-12 cm3/molecule-sec
Half-Life = 0.340 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 4.080 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi): 1
(Junge,Mackay)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 3489
Log Koc: 3.543

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates from Log Kow (BCFWIN v2.17):

Log BCF from regression-based method = 1.850 (BCF = 70.79)
log Kow used: 2.15 (estimated)

Volatilization from Water:

Henry LC: 2.86E-009 atm-m3/mole (estimated by Bond SAR Method)

Half-Life from Model River: 3.733E+005 hours
(1.555E+004 days)

Half-Life from Model Lake : 4.072E+006 hours
(1.697E+005 days)

Removal In Wastewater Treatment:

Total removal: 1.95 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.86 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.595	8.16	1000
Water	35.6	360	1000
Soil	63.7	720	1000
Sediment	0.0814	3.24e+003	0

Persistence Time: 450 hr



**Environmental
Partitioning**
