

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM : 1,2-Benzenedicarboxylic acid
CAS NUM: 000088-99-3
MOL FOR: C8 H6 O4
MOL WT : 166.13

----- 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) = 1.07
Log Kow (Exper. database match) = 0.73
Exper. Ref: Hansch,C et al. (1995)

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

Boiling Pt (deg C): 351.37 (Adapted Stein & Brown method)
Melting Pt (deg C): 126.58 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 7.67E-007 (Modified Grain method)
MP (exp database): 230 dec deg C
VP (exp database): 6.36E-07 mm Hg at 25 deg C
Subcooled liquid VP: 6.78E-005 mm Hg (25 deg C, exp database
VP)

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

Water Solubility at 25 deg C (mg/L): 1.526e+004
log Kow used: 0.73 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 7010 mg/L (25 deg C)
Exper. Ref: YALKOWSKY,SH & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 29678 mg/L
Wat Sol (Exper. database match) = 7010.00
Exper. Ref: YALKOWSKY,SH & DANNENFELSER,RM (1992)

ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:
Neutral Organics-acid

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 2.18E-012 atm-m3/mole
Group Method: 3.88E-013 atm-m3/mole
Henrys LC [VP/WSol estimate using EPI values]: 1.099E-011 atm-
m3/mole

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

Log Kow used: 0.73 (exp database)
Log Kaw used: -10.050 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 10.780
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 1.0222
Biowin2 (Non-Linear Model) : 0.9959
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.0078 (weeks)
Biowin4 (Primary Survey Model) : 3.6235 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 1.0047
Biowin6 (MITI Non-Linear Model): 0.9569
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.9855
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): 0.00904 Pa (6.78E-005 mm Hg)

Log Koa (Koawin est): 10.780

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

Mackay model : 0.000332

Octanol/air (Koa) model: 0.0148

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.0118

Mackay model : 0.0259

Octanol/air (Koa) model: 0.542

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

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 1.2370 E-12 cm³/molecule-sec

Half-Life = 8.647 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 103.764 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi): 0.0189

(Junge,Mackay)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 73.06

Log Koc: 1.864

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 = 0.500 (BCF = 3.162)

log Kow used: 0.73 (expkow database)

Volatilization from Water:

Henry LC: 3.88E-013 atm-m³/mole (estimated by Group SAR Method)

Half-Life from Model River: 1.945E+009 hours (8.104E+007 days)

Half-Life from Model Lake : 2.122E+010 hours (8.841E+008 days)

Removal In Wastewater Treatment:

Total removal: 1.87 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.78 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 | 9.9e-006 | 208 | 1000 |
| Water | 36.4 | 360 | 1000 |
| Soil | 63.5 | 720 | 1000 |
| Sediment | 0.07 | 3.24e+003 | 0 |

Persistence Time: 597 hr



**Environmental
Partitioning**
