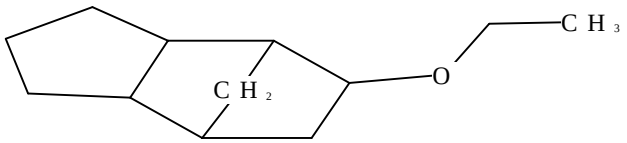

ECOSAR Version 1.11 Results Page

SMILES : CCOC1CC2CC1C3CCCC23
CHEM : PI1525
CAS Num: 1897392-68-5
ChemID1:
MOL FOR: C12 H20 O1
MOL WT : 180.29
Log Kow: 3.247 (EPISuite Kowwin v1.68 Estimate)
Log Kow: 4.020 (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 20.25 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 45.9 (mg/L, User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 4.020 (User Entered)
Wat Sol: 45.9 (mg/L, User Entered)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Neutral Organics

Note: SARs use Entered MW (180.29) instead of SMILES MW (180.29)

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics	Fish	96-hr	LC50	2.272
Neutral Organics	Daphnid	48-hr	LC50	1.555
Neutral Organics	Green Algae	96-hr	EC50	2.504
Neutral Organics	Fish		ChV	0.277
Neutral Organics	Daphnid		ChV	0.255
Neutral Organics	Green Algae		ChV	0.993
Neutral Organics	Fish (SW)	96-hr	LC50	2.895
Neutral Organics	Mysid	96-hr	LC50	0.548
Neutral Organics	Fish (SW)		ChV	1.079
Neutral Organics	Mysid (SW)		ChV	0.026
Neutral Organics	Earthworm	14-day	LC50	193.507 *

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)