Desphenyl chloridazon c4h4cln3o structure

Contents

- Safety:

Molecular Formula	$C_4H_4ClN_3O$
Average mass	145. 547 Da
Density	1. 8±0. 1 g/cm ^{3}
Boiling Point	
Flash Point	
Molar Refractivity	31. 9±0. 5 cm ^{3}
Polarizability	12. 6±0. 5 10^{-24} cm ^{3}
Surface Tension	71. 2±7. 0 dyne/cm
Molar Volume	81. 0±7. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon

- Predicted – Mcule
- Experimental Physico-chemical Properties
  - **Experimental Melting Point:**

    297-300

    °CLabNetworkLN00239928

- Miscellaneous
  - **Appearance:**

    Not AvailableNovochemy[NC-

    24054]

  - **Safety:**

    20/21/22Novochemy[N

    C-24054]

    20/21/36/37/39Novoch

    emy[NC-24054]

    GHS07;

    GHS09Novochemy[NC-

    24054]

    H332;

    H403Novochemy[NC-

    24054]

    P332+P313;

P305+P351+P338Novochemy[NC-24054]

R52/53Novochemy[NC-24054]

WarningNovochemy[NC-24054]

Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

Density:	1. 8±0. 1 g/cm ^{3}
Boiling Point:	
Vapour Pressure:	
Enthalpy of Vaporization:	
Flash Point:	
Index of Refraction:	1. 718
Molar Refractivity:	31. 9±0. 5 cm ^{3}
#H bond acceptors:	4
#H bond donors:	3
#Freely Rotating Bonds:	0

#Rule of 5 Violations:	0
ACD/LogP:	-1. 14
ACD/LogD (pH 5. 5):	-0. 63
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	10. 79
ACD/LogD (pH 7. 4):	-0. 63
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	10. 75
Polar Surface Area:	67 $Å^2$
Polarizability:	12. 6±0. 5 10^{-24} cm^3
Surface Tension:	71. 2±7. 0 dyne/cm
Molar Volume:	81. 0±7. 0 cm^3

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = -1. 59Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 362. 79 (Adapted Stein & Brown method)Melting Pt (deg C): 142. 61 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 23E-006 (Modified Grain method)Subcooled liquid VP: 6. 55E-005 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): 8. 782e+004log Kow used: -1. 59 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHydrazinesVinyl/Allyl HalidesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 27E-012 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 9. 225E-012 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 59 (KowWin est)Log Kaw used: -10. 285 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 695Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7207Biowin2 (Non-Linear Model) : 0. 5496Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7288 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5804 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3260Biowin6 (MITI Non-Linear Model): 0. 0613Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 0382Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 00873 Pa (6. 55E-005 mm Hg)Log Koa (Koawin est): 8. 695Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 000344 Octanol/air (Koa) model: 0. 000122 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0123 Mackay model : 0. 0267 Octanol/air (Koa) model: 0. 00964 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 33. 2910 E-12 cm3/molecule-secHalf-Life = 0. 321 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 855 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 162663 E-17 cm3/molecule-secHalf-Life = 7. 045 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 0. 0195 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 85Log Koc: 1. 929 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: -1. 59 (estimated)Volatilization from Water: Henry LC: 1. 27E-012 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 5. 562E+008 hours (2. 317E+007 days)Half-Life from Model Lake : 6. 067E+009 hours (2. 528E+008 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 75 percentTotal 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 1. 81e-005 7. 37 1000 Water 46. 4 900 1000 Soil 53. 5 1. 8e+003 1000 Sediment 0. 0891 8. 1e+003 0 Persistence Time: 973 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop