1,4-di(p-toluidino)anthraquinone c28h22n2o2 structure

Contents

Molecular Formula	$C_{28}H_{22}N_2O_2$
Average mass	418. 487 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	633. 8±55. 0 °C at 760 mmHg
Flash Point	197. 0±31. 7 °C
Molar Refractivity	127. 1±0. 3 cm ^{3}
Polarizability	50. 4±0. 5 10^{-24} cm ^{3}
Surface Tension	63. 0±3. 0 dyne/cm
Molar	323. 7±3. 0

Volume cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties
    - **Experimental Melting Point:**

      218 °CJean-

      Claude Bradley

      Open Melting

      Point

      Dataset17431

- Miscellaneous
    - **Safety:**

      IRRITANTMatrix

      Scientific09953

      8

- Gas Chromatography
    - **Retention Index (Kovats):**

      3953

      (estimated

with error:

89)NIST

Spectramainlib

_239577

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

Density:	1. 3±0. 1 g/cm ^{3}
Boiling Point:	633. 8±55. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 9 mmHg at 25°C
Enthalpy of Vaporization:	93. 7±3. 0 kJ/mol
Flash Point:	197. 0±31. 7 °C
Index of Refraction:	1. 714
Molar Refractivity:	127. 1±0. 3 cm ^{3}
#H bond acceptors:	4
#H bond donors:	2
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	1
ACD/LogP:	5. 41

ACD/LogD (pH 5. 5):	5. 80
ACD/BCF (pH 5. 5):	14934. 81
ACD/KOC (pH 5. 5):	33843. 83
ACD/LogD (pH 7. 4):	5. 80
ACD/BCF (pH 7. 4):	14934. 86
ACD/KOC (pH 7. 4):	33843. 94
Polar Surface Area:	58 $Å^2$
Polarizability:	50. 4±0. 5 10^{-24} cm^3
Surface Tension:	63. 0±3. 0 dyne/cm
Molar Volume:	323. 7±3. 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) = 8. 69Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 598. 47 (Adapted Stein & Brown method)Melting Pt (deg C): 258. 60 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 7. 05E-013 (Modified Grain method)MP (exp database): 218 deg CSubcooled liquid VP: 8. 09E-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): 6. 975e-006log Kow used: 8. 69 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 8. 5841e-005 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 47E-016 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 5. 566E-008 atm-m3/moleLog Octanol-Air

Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 8. 69 (KowWin est)Log Kaw used: -14. 221 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 22. 911Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2038Biowin2 (Non-Linear Model) : 0. 0015Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 8098 (months)Biowin4 (Primary Survey Model) : 2. 8457 (weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 4148Biowin6 (MITI Non-Linear Model): 0. 0003Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -2. 5829Ready 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): 1. 08E-008 Pa (8. 09E-011 mm Hg)Log Koa (Koawin est): 22. 911Kp (particle/gas partition coef. (m3/ug)): Mackay model : 278 Octanol/air (Koa) model: 2E+010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1 Mackay model : 1 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 200. 2720 E-12 cm3/molecule-secHalf-Life = 0. 053 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 641 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 3. 952E+005Log Koc: 5. 597 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. 661 (BCF = 45. 79)log Kow used: 8. 69 (estimated)Volatilization from Water: Henry LC: 1. 47E-016 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 8. 148E+012 hours (3. 395E+011 days)Half-Life from Model Lake : 8. 889E+013 hours (3. 704E+012 days)Removal In Wastewater Treatment: Total removal: 94. 03 percentTotal biodegradation: 0. 78 percentTotal sludge adsorption: 93. 25 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 2. 01e-006 1. 28 1000 Water 1. 15 1. 44e+003 1000 Soil 42. 1 2. 88e+003 1000 Sediment 56. 7 1. 3e+004 0 Persistence Time: 6. 25e+003 hr

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