

# [1,4-di(p-toluidino)anthraquinone c28h22n2o2 structure](https://assignbuster.com/14-dip-toluidinoanthraquinone-c28h22n2o2-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 28 H 22 N 2 O 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 Volume  | 323. 7±3. 0 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 Scientific099538  |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 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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