

# [2,7-naphthalenedicarboxylic acid c12h8o4 structure](https://assignbuster.com/27-naphthalenedicarboxylic-acid-c12h8o4-structure/)

Contents

* Safety:

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| Molecular Formula  | C 12 H 8 O 4  |
| Average mass  | 216. 189 Da  |
| Density  | 1. 5±0. 1 g/cm 3  |
| Boiling Point  | 437. 3±25. 0 °C at 760 mmHg  |
| Flash Point  | 232. 4±19. 7 °C  |
| Molar Refractivity  | 58. 0±0. 3 cm 3  |
| Polarizability  | 23. 0±0. 5 10 -24 cm 3  |
| Surface Tension  | 73. 7±3. 0 dyne/cm  |
| Molar Volume  | 148. 6±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Miscellaneous

## Appearance:

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| Not AvailableNovochemy[NC-28554]  |

## Safety:

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| 20/21/22Novochemy[NC-28554]  |
| 20/21/36/37/39Novochemy[NC-28554]  |
| GHS07; GHS09Novochemy[NC-28554]  |
| H332; H403Novochemy[NC-28554]  |
| P309+P311; P211; P242Novochemy[NC-28554]  |
| WarningNovochemy[NC-28554]  |
| XnNovochemy[NC-28554]  |

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

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| Density:  | 1. 5±0. 1 g/cm 3  |
| Boiling Point:  | 437. 3±25. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±1. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 73. 1±3. 0 kJ/mol  |
| Flash Point:  | 232. 4±19. 7 °C  |
| Index of Refraction:  | 1. 708  |
| Molar Refractivity:  | 58. 0±0. 3 cm 3  |
| #H bond acceptors:  | 4  |
| #H bond donors:  | 2  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

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| ACD/LogP:  | 2. 80  |
| ACD/LogD (pH 5. 5):  | -0. 22  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 01  |
| ACD/LogD (pH 7. 4):  | -1. 62  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 1. 00  |
| Polar Surface Area:  | 75 Å 2  |
| Polarizability:  | 23. 0±0. 5 10 -24 cm 3  |
| Surface Tension:  | 73. 7±3. 0 dyne/cm  |
| Molar Volume:  | 148. 6±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) = 2. 93Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 422. 27 (Adapted Stein & Brown method)Melting Pt (deg C): 176. 29 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 6. 4E-008 (Modified Grain method)Subcooled liquid VP: 2. 38E-006 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): 113log Kow used: 2. 93 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 33. 317 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 13E-013 atm-m3/moleGroup Method: 2. 68E-014 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 611E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 93 (KowWin est)Log Kaw used: -11. 060 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 13. 990Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9983Biowin2 (Non-Linear Model) : 0. 9917Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8971 (weeks )Biowin4 (Primary Survey Model) : 3. 5513 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 8722Biowin6 (MITI Non-Linear Model): 0. 8693Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 7947Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 000317 Pa (2. 38E-006 mm Hg)Log Koa (Koawin est ): 13. 990Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00945 Octanol/air (Koa) model: 24 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 255 Mackay model : 0. 431 Octanol/air (Koa) model: 0. 999 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 3. 2219 E-12 cm3/molecule-secHalf-Life = 3. 320 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 39. 837 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 343 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 794. 8Log Koc: 2. 900 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: 2. 93 (estimated)Volatilization from Water: Henry LC: 2. 68E-014 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 3. 212E+010 hours (1. 338E+009 days)Half-Life from Model Lake : 3. 504E+011 hours (1. 46E+010 days)Removal In Wastewater Treatment: Total removal: 5. 14 percentTotal biodegradation: 0. 12 percentTotal sludge adsorption: 5. 02 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 6. 86e-007 79. 7 1000 Water 17 360 1000 Soil 82. 7 720 1000 Sediment 0. 25 3. 24e+003 0 Persistence Time: 772 hr

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