

2,7-

naphthalenedicarboxylic acid c₁₂h₈o₄
structure



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Contents

- Safety:

Molecular
Formula $C_{12}H_8O_4$

Average mass 216. 189 Da

Density $1. 5 \pm 0. 1 \text{ g/cm}^3$

Boiling Point $437. 3 \pm 25. 0 \text{ }^\circ\text{C}$ at 760
mmHg

Flash Point $232. 4 \pm 19. 7 \text{ }^\circ\text{C}$

Molar
Refractivity $58. 0 \pm 0. 3 \text{ cm}^3$

Polarizability $23. 0 \pm 0. 5 \cdot 10^{-24} \text{ cm}^3$

Surface Tension $73. 7 \pm 3. 0 \text{ dyne/cm}$

Molar Volume $148. 6 \pm 3. 0 \text{ cm}^3$

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

- Miscellaneous

- **Appearance:**

Not AvailableNovochemistry[NC-28554]

- **Safety:**

20/21/22Novochemistry[NC-28554]

20/21/36/37/39Novochemistry[NC-28554]

GHS07; GHS09Novochemistry[NC-28554]

H332; H403Novochemistry[NC-28554]

P309+P311; P211;

P242Novochemistry[NC-28554]

WarningNovochemistry[NC-28554]

XnNovochemistry[NC-28554]

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

Density: 1.5±0.1 g/cm³

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

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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
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: $23.0 \pm 0.5 \times 10^{-24} \text{ cm}^3$

Surface Tension: $73.7 \pm 3.0 \text{ dyne/cm}$

Molar Volume: $148.6 \pm 3.0 \text{ cm}^3$

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. 93 Boiling 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): 113 log Kow used: 2. 93 (estimated) no-melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 33. 317 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics-acid Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 13E-013 atm-m³/mole Group Method: 2. 68E-014 atm-m³/mole Henrys LC [VP/WSol estimate using EPI values]: 1. 611E-010 atm-m³/mole Log 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. 990 Log Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9983 Biowin2 (Non-Linear Model) : 0. 9917 Expert 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. 8722 Biowin6 (MITI Non-Linear Model): 0. 8693 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 7947 Ready Biodegradability Prediction: YES Hydrocarbon 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. 990 Kp (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/mole-sec Half-Life = 3. 320 Days (12-hr day; 1. 5E6 OH/cm³) Half-Life = 39. 837 Hrs Ozone Reaction: No Ozone Reaction Estimation Fraction sorbed to airborne particulates (phi): 0. 343 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 794. 8 Log 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.

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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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