

# [Phthalic anhydride c8h4o3 structure](https://assignbuster.com/phthalic-anhydride-c8h4o3-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula | C 8 H 4 O 3 |
| Average mass | 148. 116 Da |
| Density | 1. 4±0. 1 g/cm 3 |
| Boiling Point | 295. 0±0. 0 °C at 760 mmHg |
| Flash Point | 139. 7±15. 9 °C |
| Molar Refractivity | 35. 7±0. 3 cm 3 |
| Polarizability | 14. 1±0. 5 10 -24 cm 3 |
| Surface Tension | 58. 1±3. 0 dyne/cm |
| Molar Volume | 102. 6±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 131-133 °CAlfa Aesar |
| 130-134 °CAlfa Aesar |
| 129-133 °CMerck Millipore1922, 800592 |
| 130. 8 °CJean-Claude Bradley Open Melting Point Dataset21060 |
| 132 °CJean-Claude Bradley Open Melting Point Dataset8284 |
| 131-133 °CAlfa Aesar41771 |
| 130-134 °CAlfa AesarA14955 |
| 131-134 °CSynQuest56195, 2H26-1-01 |
| 130-132 °CLabNetworkLN00196238 |

## Experimental Boiling Point:

|  |
| --- |
| 295 °C (Sublimes)Alfa Aesar |
| 563 F (295 °C)NIOSHTI3150000 |
| 295 °C (Sublimes)Alfa Aesar41771, A14955 |
| 284 °CSynQuest56195, 2H26-1-01 |
| 284 °CLabNetworkLN00196238 |

## Experimental Ionization Potent:

|  |
| --- |
| 10 EvNIOSHTI3150000 |

## Experimental Vapor Pressure:

|  |
| --- |
| 0. 0015 mmHgNIOSHTI3150000 |

## Experimental Flash Point:

|  |
| --- |
| 152 °CAlfa Aesar |
| 305 F (151. 6667 °C)NIOSHTI3150000 |
| 152 °CAlfa Aesar |
| 152 °F (66. 6667 °C)Alfa Aesar41771, A14955 |
| 152 °CLabNetworkLN00196238 |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLSynQuest2H26-1-01 |
| 1. 53 g/mLAlfa Aesar41771, A14955 |
| 1. 53 g/mLSynQuest2H26-1-01 |
| 1. 53 g/lFluorochem093917 |

## Experimental Solubility:

|  |
| --- |
| 0. 6%NIOSHTI3150000 |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 131-134 °CJ&K Scientific906637, 510421 |
| 131 °CTCI |
| 131 °CTCIP1614 |

* Miscellaneous

## Appearance:

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| White solid (flake) or a clear, colorless, mobile liquid (molten) with a characteristic, acrid odor. NIOSHTI3150000 |

## Safety:

|  |
| --- |
| 22-37/38-41-42/43Alfa Aesar41771, A14955 |
| 23-24/25-26-37/39-46Alfa Aesar41771, A14955 |
| 8Alfa Aesar41771, A14955 |
| DangerAlfa Aesar41771, A14955 |
| DANGER: CORROSIVE, burns skin and eyesAlfa AesarA14955 |
| H334-H318-H302-H335-H315-H317Alfa Aesar41771, A14955 |
| Harmful/Irritant/Dangerous for the Environment/Skin and respiratory sensitizerSynQuest2H26-1-01, 56195 |
| IRRITANTMatrix Scientific099103 |
| P285-P261-P280-P305+P351+P338-P405-P501aAlfa Aesar41771, A14955 |
| R20/21/22, R36/37/38, R42, R43, R52SynQuest2H26-1-01, 56195 |
| S13, S22, S24/25, S26, S36/37/39, S45, S61SynQuest2H26-1-01, 56195 |
| WARNING: Irritates skin and eyesAlfa Aesar41771 |
| WARNING: Irritates skin and eyes, harmful if swallowedAlfa Aesar41771, A14955 |
| XnAbblis ChemicalsAB1002188 |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Soap wash promptly Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHTI3150000 |

## Exposure Routes:

|  |
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| inhalation, ingestion, skin and/or eye contactNIOSHTI3150000 |

## Symptoms:

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| Irritation eyes, skin, upper respiratory system; conjunctivitis; nasal ulcer bleeding; bronchitis, bronchial asthma; dermatitis; in animals: liver, kidney damageNIOSHTI3150000 |

## Target Organs:

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| Eyes, skin, respiratory system, liver, kidneysNIOSHTI3150000 |

## Incompatibility:

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| Strong oxidizers, water [Note: Converted to phthalic acid in hot water.]NIOSHTI3150000 |

## Personal Protection:

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| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet or contaminated Change: DailyNIOSHTI3150000 |

## Exposure Limits:

|  |
| --- |
| NIOSH REL : TWA 6 mg/m 3 (1 ppm) OSHA PEL ?: TWA 12 mg/m 3 (2 ppm)NIOSHTI3150000 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1443 (estimated with error: 89)NIST Spectramainlib\_133911, replib\_160694, replib\_227884 |

## Retention Index (Lee):

|  |
| --- |
| 225. 33 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 310 C; End time: 10 min; Start time: 1. 5 min; CAS no: 85449; Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Pedersen, D. U.; Durant, J. L.; Taghizadeh, K.; Hemond, H. F.; Lafleur, A. L.; Cass, G. R., Human cell mutagenes in respirable airborne particles from the Northeastern United States. 2. Quantification of mutagenes and other organic compounds., Environ. Sci. Technol., 39(24), 2005, 9547-9560.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1308 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 280 C; End time: 10 min; Start time: 0. 5 min; CAS no: 85449; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Guillen, M. D.; Manzanos, M. J., Study of the volatile composition of an aqueous oak smoke preparation, Food Chem., 79, 2002, 283-292.)NIST Spectranist ri |

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

|  |  |
| --- | --- |
| Density: | 1. 4±0. 1 g/cm 3 |
| Boiling Point: | 295. 0±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 6 mmHg at 25°C |
| Enthalpy of Vaporization: | 53. 5±3. 0 kJ/mol |
| Flash Point: | 139. 7±15. 9 °C |
| Index of Refraction: | 1. 613 |
| Molar Refractivity: | 35. 7±0. 3 cm 3 |
| #H bond acceptors: | 3 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 0 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 1. 60 |
| ACD/LogD (pH 5. 5): | 1. 42 |
| ACD/BCF (pH 5. 5): | 7. 10 |
| ACD/KOC (pH 5. 5): | 141. 53 |
| ACD/LogD (pH 7. 4): | 1. 42 |
| ACD/BCF (pH 7. 4): | 7. 10 |
| ACD/KOC (pH 7. 4): | 141. 53 |
| Polar Surface Area: | 43 Å 2 |
| Polarizability: | 14. 1±0. 5 10 -24 cm 3 |
| Surface Tension: | 58. 1±3. 0 dyne/cm |
| Molar Volume: | 102. 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. 07Log Kow (Exper. database match) = 1. 60Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 253. 03 (Adapted Stein & Brown method)Melting Pt (deg C): 21. 79 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000222 (Modified Grain method)MP (exp database): 130. 8 deg CBP (exp database): 295 deg CVP (exp database): 5. 17E-04 mm Hg at 25 deg CSubcooled liquid VP: 0. 00575 mm Hg (25 deg C, exp database VP )Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 3326log Kow used: 1. 60 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 6200 mg/L (25 deg C)Exper. Ref: TOWLE, PH ET AL. (1968)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 24982 mg/LWat Sol (Exper. database match) = 6200. 00Exper. Ref: TOWLE, PH ET AL. (1968)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 35E-006 atm-m3/moleGroup Method: IncompleteExper Database: 1. 63E-08 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 301E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 60 (exp database)Log Kaw used: -6. 176 (exp database)Log Koa (KOAWIN v1. 10 estimate): 7. 776Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6770Biowin2 (Non-Linear Model) : 0. 7121Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8718 (weeks )Biowin4 (Primary Survey Model) : 3. 6340 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3044Biowin6 (MITI Non-Linear Model): 0. 2193Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4544Ready 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. 767 Pa (0. 00575 mm Hg)Log Koa (Koawin est ): 7. 776Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 91E-006 Octanol/air (Koa) model: 1. 47E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000141 Mackay model : 0. 000313 Octanol/air (Koa) model: 0. 00117 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 7492 E-12 cm3/molecule-secHalf-Life = 14. 276 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000227 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 10. 84Log Koc: 1. 035 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. 532 (BCF = 3. 404)log Kow used: 1. 60 (expkow database)Volatilization from Water: Henry LC: 1. 63E-008 atm-m3/mole (Henry experimental database)Half-Life from Model River: 4. 372E+004 hours (1822 days)Half-Life from Model Lake : 4. 77E+005 hours (1. 988E+004 days)Removal In Wastewater Treatment: Total removal: 2. 01 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 91 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 0. 321 343 1000 Water 28. 2 360 1000 Soil 71. 4 720 1000 Sediment 0. 0709 3. 24e+003 0 Persistence Time: 645 hr

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* 1-Click Scaffold Hop