Phthalic anhydride c8h4o3 structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_8H_4O_3$
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

°CLabNetworkLN001962

38

- **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

°CLabNetworkLN001962

38

- **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:**

    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:**

  Eye: Irrigate immediately

  Skin: Soap wash

  promptly Breathing:

  Respiratory support

  Swallow: Medical

  attention

  immediatelyNIOSHTI315

0000

- **Exposure Routes:**

  inhalation, ingestion,

  skin and/or eye

  contactNIOSHTI3150000

- **Symptoms:**

  Irritation eyes, skin,

  upper respiratory

  system; conjunctivitis;

  nasal ulcer bleeding;

  bronchitis, bronchial

  asthma; dermatitis; in

  animals: liver, kidney

  damageNIOSHTI3150000

- **Target Organs:**

  Eyes, skin, respiratory

  system, liver,

  kidneysNIOSHTI3150000

- **Incompatibility:**

  Strong oxidizers, water

  [Note: Converted to

  phthalic acid in hot

water.]NIOSHTI3150000

- **Personal Protection:**

  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