4-phenylbutyric acid c10h12o2 structure

ASSIGN BUSTER

Contents

- Retention Index (Linear):

Molecular Formula	$C_{10}H_{12}O_2$
Average mass	164. 201 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	290. 7±9. 0 °C at 760 mmHg
Flash Point	187. 9±13. 9 °C
Molar Refractivity	46. 6±0. 3 cm ^{3}
Polarizability	18. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	43. 6±3. 0 dyne/cm
Molar Volume	149. 9±3. 0 cm ^{3}

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

- Experimental Physico-chemical Properties

Experimental Melting Point:

49-53 °CSynQuest

52 °CTCIP0643

49-53 °CAlfa Aesar

48 °CMolMall

48-51 °CMerck Millipore3618, 820986

48 °CJean-Claude Bradley Open Melting Point Dataset13010

52 °CJean-Claude Bradley Open Melting Point Dataset21645, 27702

51 °CJean-Claude Bradley Open Melting Point Dataset5557

49-53 °CAlfa AesarA18115

49-53 °CSynQuest62405, 2621-1-X9

50 °CBiosynthQ-200508

48 °CMolMall18169

48 °CLabNetworkLN00196776

- **Experimental Boiling Point:**

  165 deg C / 10 mm (340. 371 °C / 760 mmHg)Alfa Aesar

  165 °C / 10 mm (340. 371 °C / 760 mmHg)Alfa AesarA18115

  165 °C / 10 mmHg (340. 371 °C / 760 mmHg)SynQuest62405, 2621-1-X9

- **Experimental LogP:**

  2. 419Vitas-MSTL164372

  2. 42Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s

- **Experimental Flash Point:**

  110 °CAlfa Aesar

  110 °CAlfa Aesar

  113 °CBiosynthQ-200508

  110 °F (43. 3333 °C)Alfa AesarA18115

  113 °CSynQuest62405, 2621-1-

X9

230 °CLabNetworkLN00196776

- **Experimental Gravity:**

  113 g/mLBiosynthQ-

  200508

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    52 °CTCI

    52

    °CTCIP0643

- Miscellaneous

  - **Appearance:**

    White CrystalNovochemy[NC-

    01213]

  - **Safety:**

    20/21/36/37/39Novochemy[NC-01213]

    26-37Alfa AesarA18115

    36/37/38Alfa AesarA18115

    36/37/38Novochemy[NC-01213]

GHS07BiosynthQ-200508

GHS07; GHS09Novochemy[NC-01213]

H304; H332; H403Novochemy[NC-01213]

H315; H319; H335BiosynthQ-200508

H315-H319-H335Alfa AesarA18115

IrritantSynQuest2621-1-X9, 62405

P261; P280; P302+P352; P304+P340; P305+P351+P338; P312BiosynthQ-200508

P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA18115

P332+P313; P305+P351+P338Novochemy[NC-01213]

R52/53Novochemy[NC-01213]

WarningAlfa AesarA18115

WarningBiosynthQ-200508

WarningNovochemy[NC-01213]

WARNING: Irritates lungs, eyes, skinAlfa AesarA18115

- **Therapeutical Effect:**

  antiinflammatoryMicrosource[00

  306001]

- **Drug Status:**

  experimentalMicrosource[003

  06001]

- **Compound Source:**

  syntheticMicrosource[0030

  6001]

- Gas Chromatography

  - **Retention Index (Kovats):**

    1448 (estimated with error: 51)NIST Spectramainlib_232280, replib_6067

    replib_135631, replib_151674

  - **Retention Index (Lee):**

    244. 61 (Program type: Ramp; Column cl... (show more)ass: Standard no

    Column type: Capillary; CAS no: 1821121; Active phase: Methyl Silicone;

    type: Lee RI; Authors: Eckel, W. P.; Ross, B.; Isensee, R. K., Pentobarbital

    ground water, Ground Water, 31(5), 1993, 801-804.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

  1408. 9 (Program type: Ramp; Column cl... (show more)ass: Standard no

  Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capilla

  rate: 20 K/min; Start T: 50 C; End T: 250 C; Start time: 1 min; CAS no: 18

  Active phase: HP-1; Carrier gas: He; Data type: Normal alkane RI; Author

  Katritzky, A. R.; Ignatchenko, E. S.; Barcock, R. A.; Lobanov, V. S.; Karelso

  Prediction of gas chromatographic retention times and response factors

  general quantitative structure — property relationship treatment, Anal. C

  66, 1994, 1799-1807.)NIST Spectranist ri

- **Retention Index (Linear):**

  1417 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

  Column length: 3. 05 m; Column type: Packed; Heat rate: 10 K/min; Start

  End T: 250 C; End time: 60 min; Start time: 4 min; CAS no: 1821121; Act

  phase: SE-30; Carrier gas: He; Substrate: Supelcoport and Chromosorb; D

  type: Linear RI; Authors: Peng, C. T.; Ding, S. F.; Hua, R. L.; Yang, Z. C., P

  of Retention Indexes I. Structure-Retention Index Relationship on Apolar

  Columns, J. Chromatogr., 436, 1988, 137-172.)NIST Spectranist ri

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

Density:	1. 1±0. 1 g/cm ^{3}
Boiling Point:	290. 7±9. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 6 mmHg at 25°C

Enthalpy of Vaporization:	56. 0±3. 0 kJ/mol
Flash Point:	187. 9±13. 9 °C
Index of Refraction:	1. 535
Molar Refractivity:	46. 6±0. 3 cm^3
#H bond acceptors:	2
#H bond donors:	1
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	0
ACD/LogP:	2. 42
ACD/LogD (pH 5. 5):	1. 48
ACD/BCF (pH 5. 5):	4. 97
ACD/KOC (pH 5. 5):	64. 34
ACD/LogD (pH 7. 4):	-0. 32
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 03

Polar Surface Area:	37 Å ^{2}
Polarizability:	18. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	43. 6±3. 0 dyne/cm
Molar Volume:	149. 9±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. 78Log Kow (Exper. database match) = 2. 42Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 298. 00 (Adapted Stein & Brown method)Melting Pt (deg C): 79. 00 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00187 (Modified Grain method)MP (exp database): 52 deg CBP (exp database): 290 deg CSubcooled liquid VP: 0. 00331 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): 1394log Kow used: 2. 42 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 653. 21 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics-acidHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 79E-008 atm-m3/moleGroup Method: 1. 23E-008 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 898E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 42 (exp database)Log Kaw used: -5. 497 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 917Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9248Biowin2 (Non-Linear Model) : 0. 9758Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1481 (weeks)Biowin4 (Primary Survey Model) : 3. 9328 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4890Biowin6 (MITI Non-Linear Model): 0. 5634Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6941Ready 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. 441 Pa (0. 00331 mm Hg)Log Koa (Koawin est): 7. 917Kp (particle/gas partition coef. (m3/ug)): Mackay model : 6. 8E-006 Octanol/air (Koa) model: 2. 03E-005 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000245 Mackay model : 0. 000544 Octanol/air (Koa) model: 0. 00162 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 8. 7886 E-12 cm3/molecule-secHalf-Life = 1. 217 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 14. 604 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000394 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 89. 07Log Koc: 1. 950 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. 42 (expkow database)Volatilization from Water: Henry LC: 1. 23E-008 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 6. 1E+004 hours (2542 days)Half-Life from Model Lake : 6. 655E+005 hours (2. 773E+004 days)Removal In Wastewater Treatment: Total removal: 2. 89 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 79 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. 201 29. 2 1000 Water 19. 9 360 1000 Soil 79. 8 720 1000 Sediment 0. 122 3. 24e+003 0 Persistence Time: 705 hr

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- 1-Click Scaffold Hop