

# [4-phenylbutyric acid c10h12o2 structure](https://assignbuster.com/4-phenylbutyric-acid-c10h12o2-structure/)

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:

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| --- |
| antiinflammatoryMicrosource[00306001] |

## Drug Status:

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| --- |
| experimentalMicrosource[00306001] |

## Compound Source:

|  |
| --- |
| syntheticMicrosource[00306001] |

* 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 non-polar; Column type: Capillary; CAS no: 1821121; Active phase: Methyl Silicone; Data type: Lee RI; Authors: Eckel, W. P.; Ross, B.; Isensee, R. K., Pentobarbital found in 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 non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 20 K/min; Start T: 50 C; End T: 250 C; Start time: 1 min; CAS no: 1821121; Active phase: HP-1; Carrier gas: He; Data type: Normal alkane RI; Authors: Katritzky, A. R.; Ignatchenko, E. S.; Barcock, R. A.; Lobanov, V. S.; Karelson, M., Prediction of gas chromatographic retention times and response factors using a general quantitative structure — property relationship treatment, Anal. Chem., 66, 1994, 1799-1807.)NIST Spectranist ri |

## Retention Index (Linear):

|  |
| --- |
| 1417 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 3. 05 m; Column type: Packed; Heat rate: 10 K/min; Start T: 40 C; End T: 250 C; End time: 60 min; Start time: 4 min; CAS no: 1821121; Active phase: SE-30; Carrier gas: He; Substrate: Supelcoport and Chromosorb; Data type: Linear RI; Authors: Peng, C. T.; Ding, S. F.; Hua, R. L.; Yang, Z. C., Prediction 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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