

# [4-aminophenol c6h7no structure](https://assignbuster.com/4-aminophenol-c6h7no-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 7 NO  |
| Average mass  | 109. 126 Da  |
| Density  | 1. 2±0. 1 g/cm 3  |
| Boiling Point  | 282. 0±23. 0 °C at 760 mmHg  |
| Flash Point  | 124. 3±22. 6 °C  |
| Molar Refractivity  | 32. 4±0. 3 cm 3  |
| Polarizability  | 12. 8±0. 5 10 -24 cm 3  |
| Surface Tension  | 57. 4±3. 0 dyne/cm  |
| Molar Volume  | 90. 1±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 187 °CTCIA0384  |
| 186-190 °CAlfa Aesar  |
| 188-190 °COxford University Chemical Safety Data (No longer updated)More details  |
| 186-191 °CMerck Millipore4799, 845129  |
| 189 °CJean-Claude Bradley Open Melting Point Dataset13409, 15441  |
| 187. 5 °CJean-Claude Bradley Open Melting Point Dataset22450  |
| 188 °CJean-Claude Bradley Open Melting Point Dataset4605  |
| 186-190 °CAlfa AesarA13581  |
| 185-190 °CSynQuest4656-1-14  |
| 188 °CLabNetworkLN00192892  |
| 155 °C (Decomposes)LabNetworkLN00192892  |

## Experimental Boiling Point:

|  |
| --- |
| 284 °C (Decomposes)Alfa Aesar  |
| 284 °C (Decomposes)Alfa AesarA13581  |
| 284 °C (Decomposes)SynQuest4656-1-14  |
| 168 °CBiosynthQ-200462  |
| 284 °CLabNetworkLN00192892  |

## Experimental LogP:

|  |
| --- |
| -0. 287Vitas-MSTK286017  |
| 0. 04Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s  |

## Experimental Flash Point:

|  |
| --- |
| 195 °CAlfa Aesar  |
| 195 °COxford University Chemical Safety Data (No longer updated)More details  |
| 195 °CAlfa Aesar  |
| 109 °CBiosynthQ-200462  |
| 195 °F (90. 5556 °C)Alfa AesarA13581  |
| 195 °CSynQuest4656-1-14  |
| 189 °CLabNetworkLN00192892  |

## Experimental Gravity:

|  |
| --- |
| 1. 22 g/mLBiosynthQ-200462  |
| 1. 29 g/mLAlfa AesarA13581  |
| 1. 29 g/mLSynQuest4656-1-14  |
| 109 g/mLBiosynthQ-200462  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 187 °CTCI  |
| 187 °CTCIA0384  |

* Miscellaneous

## Appearance:

|  |
| --- |
| Not AvailableNovochemy[NC-30658]  |
| off-white crystals or powderOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Stable, though may discolour in air. Incompatiblewith acids, chloroformates, strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 375 mg kg-1, IPR-RAT LD50 465 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 20/21/22Novochemy[NC-30658]  |
| 20/21/36/37/39Novochemy[NC-30658]  |
| 20/22-68-50/53Alfa AesarA13581  |
| 28-36/37-60-61Alfa AesarA13581  |
| 6. 1Alfa AesarA13581  |
| GHS07BiosynthQ-200462  |
| GHS07; GHS09Novochemy[NC-30658]  |
| H302BiosynthQ-200462  |
| H332; H403Novochemy[NC-30658]  |
| H341-H400-H410-H302-H332Alfa AesarA13581  |
| P280h-P273-P302+P352-P501aAlfa AesarA13581  |
| P301+P312; P330BiosynthQ-200462  |
| P309+P311; P211; P242Novochemy[NC-30658]  |
| R52/53Novochemy[NC-30658]  |
| Safety glasses, gloves, good ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |
| Toxic/Harmful/Mutagenic/Air Sensitive/Store under ArgonSynQuest4656-1-14  |
| WarningAlfa AesarA13581  |
| WarningBiosynthQ-200462  |
| WarningNovochemy[NC-30658]  |
| WARNING: Irreversible damage risk, protect skin/eyes/lungs. Alfa AesarA13581  |
| Xn, NAbblis ChemicalsAB1009438  |

## Target Organs:

|  |
| --- |
| ROS inhibitorTargetMolT0648  |

## Bio Activity:

|  |
| --- |
| Free radical scavengersTargetMolT0648  |
| Immunology/InflammationTargetMolT0648  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1213 (estimated with error: 89)NIST Spectramainlib\_228504, replib\_290646, replib\_155803  |
| 1314 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column length: 2. 9 m; Column type: Packed; CAS no: 123308; Active phase: SE-30; Substrate: Chromosorb W HMDS (80-100 mesh); Data type: Kovats RI; Authors: Grzybowski, J.; Lamparczyk, H.; Nasal, A.; Radecki, A., Relationship between the retention indices of phenols on polar and non-polar stationary phases, J. Chromatogr., 196, 1980, 217-223.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1314 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 123308; Active phase: SE-30; Data type: Normal alkane RI; Authors: Peterson, K. L., Counter-Propagation Neural Networks in the Modeling and Prediction of Kovats Indices for Substituted Phenols, Anal. Chem., 64(4), 1992, 379-386.)NIST Spectranist ri  |
| 1265 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 123308; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 1265 (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: 123308; 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. 2±0. 1 g/cm 3  |
| Boiling Point:  | 282. 0±23. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 6 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 54. 2±3. 0 kJ/mol  |
| Flash Point:  | 124. 3±22. 6 °C  |
| Index of Refraction:  | 1. 637  |
| Molar Refractivity:  | 32. 4±0. 3 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 3  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | -0. 29  |
| ACD/LogD (pH 5. 5):  | -0. 04  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 18. 11  |
| ACD/LogD (pH 7. 4):  | 0. 16  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 28. 98  |
| Polar Surface Area:  | 46 Å 2  |
| Polarizability:  | 12. 8±0. 5 10 -24 cm 3  |
| Surface Tension:  | 57. 4±3. 0 dyne/cm  |
| Molar Volume:  | 90. 1±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) = 0. 24Log Kow (Exper. database match) = 0. 04Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 241. 84 (Adapted Stein & Brown method)Melting Pt (deg C): 53. 57 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 27E-005 (Modified Grain method)MP (exp database): 187. 5 deg CBP (exp database): 284 deg CVP (exp database): 4. 00E-05 mm Hg at 25 deg CSubcooled liquid VP: 0. 00162 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): 1. 012e+005log Kow used: 0. 04 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 6000 mg/L (25 deg C)Exper. Ref: DUNN, SA (1954)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 41737 mg/LWat Sol (Exper. database match) = 6000. 00Exper. Ref: DUNN, SA (1954)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesPhenolsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 98E-010 atm-m3/moleGroup Method: 2. 68E-010 atm-m3/moleExper Database: 9. 57E-10 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 640E-011 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 04 (exp database)Log Kaw used: -7. 408 (exp database)Log Koa (KOAWIN v1. 10 estimate): 7. 448Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5777Biowin2 (Non-Linear Model) : 0. 6132Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8794 (weeks )Biowin4 (Primary Survey Model) : 3. 6216 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3269Biowin6 (MITI Non-Linear Model): 0. 2927Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2573Ready 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. 216 Pa (0. 00162 mm Hg)Log Koa (Koawin est ): 7. 448Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 39E-005 Octanol/air (Koa) model: 6. 89E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000501 Mackay model : 0. 00111 Octanol/air (Koa) model: 0. 000551 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 74. 2471 E-12 cm3/molecule-secHalf-Life = 0. 144 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 729 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 000806 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 72. 53Log Koc: 1. 861 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: 0. 04 (expkow database)Volatilization from Water: Henry LC: 9. 57E-010 atm-m3/mole (Henry experimental database)Half-Life from Model River: 6. 391E+005 hours (2. 663E+004 days)Half-Life from Model Lake : 6. 972E+006 hours (2. 905E+005 days)Removal In Wastewater Treatment: Total removal: 1. 85 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 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. 0217 3. 46 1000 Water 38. 8 360 1000 Soil 61. 1 720 1000 Sediment 0. 0717 3. 24e+003 0 Persistence Time: 565 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop