4-aminophenol c6h7no structure

Contents

- Retention Index (Linear):

Molecular Formula	C_6H_7NO
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      188-190 °COxford University Chemical Safety Data (No longer updated)More details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

°CLabNetworkLN001928

92

155 °C

(Decomposes)LabNetwo

rkLN00192892

- **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

°CLabNetworkLN001928

92

- **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