

# [Benzoquinone c6h4o2 structure](https://assignbuster.com/benzoquinone-c6h4o2-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 4 O 2  |
| Average mass  | 108. 095 Da  |
| Density  | 1. 3±0. 1 g/cm 3  |
| Boiling Point  | 174. 0±15. 0 °C at 760 mmHg  |
| Flash Point  | 59. 3±17. 4 °C  |
| Molar Refractivity  | 27. 1±0. 3 cm 3  |
| Polarizability  | 10. 8±0. 5 10 -24 cm 3  |
| Surface Tension  | 47. 8±3. 0 dyne/cm  |
| Molar Volume  | 86. 0±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 113 °CTCIB0887, B0089  |
| 112-115 °CAlfa Aesar  |
| 113-115 °COxford University Chemical Safety Data (No longer updated)More details  |
| 115. 7 °CLKT Labs[B1853]  |
| 112-115 °CMerck Millipore1360, 802410  |
| 115. 7 °CJean-Claude Bradley Open Melting Point Dataset21672  |
| 114 °CJean-Claude Bradley Open Melting Point Dataset13404, 14961, 8217  |
| 112-115 °CAlfa AesarA13162  |
| 113-115 °COakwood094629  |
| 113 °CBiosynthJ-503966  |
| 107-111 °C (Decomposes)LabNetworkLN00194634  |
| 115. 7 °CFooDBFDB005755  |

## Experimental Boiling Point:

|  |
| --- |
| 180 °C (Sublimes)Alfa Aesar  |
| 180 °COxford University Chemical Safety Data (No longer updated)More details  |
| 180 °C (Sublimes)Alfa AesarA13162  |
| 174 °CBiosynthJ-503966  |
| 293 °CLabNetworkLN00194634  |

## Experimental Ionization Potent:

|  |
| --- |
| 9. 68 EvNIOSHDK2625000  |

## Experimental LogP:

|  |
| --- |
| 0. 265Vitas-MSTK398389  |

## Experimental Flash Point:

|  |
| --- |
| 77 °CAlfa Aesar  |
| 100-200 F (37. 7778-93. 3333 °C)NIOSHDK2625000  |
| 77 °CAlfa Aesar  |
| 77 °F (25 °C)Alfa AesarA13162  |
| 38 °CLabNetworkLN00194634  |

## Experimental Gravity:

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| --- |
| 1. 318 g/mLAlfa AesarA13162  |
| 59. 3 g/mLBiosynthJ-503966  |

## Experimental Solubility:

|  |
| --- |
| -0. 99Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s  |
| SlightNIOSHDK2625000  |
| Slightly soluble in water. Soluble in alcohol, ether or alkalies. LKT Labs[B1853]  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 113 °CTCI  |
| 113 °CTCIB0887, B0089  |

* Miscellaneous

## Appearance:

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| --- |
| gold powderOxford University Chemical Safety Data (No longer updated)More details  |
| Pale-yellow solid with an acrid, chlorine-like odor. NIOSHDK2625000  |

## Stability:

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| --- |
| Stable, but light sensitive. Incompatible with strong oxidizing agents. Flammable. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 100 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 23/25-36/37/38-50Alfa AesarA13162  |
| 23/25-36/37/38-50LKT Labs[B1853]  |
| 26-28-45-61Alfa AesarA13162  |
| 6. 1Alfa AesarA13162  |
| DangerAlfa AesarA13162  |
| DANGER: POISON, severe eye, skin and lung irritantAlfa AesarA13162  |
| H301-H331-H400-H315-H319-H335Alfa AesarA13162  |
| H331 H301 H315 H319 H335LKT Labs[B1853]  |
| P280h-P273-P305+P351+P338-P309-P310-P302+P352Alfa AesarA13162  |
| Safety glasses, gloves. Effective ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |
| T, NLKT Labs[B1853]  |
| T, NAbblis ChemicalsAB1002099  |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Soap wash immediately Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHDK2625000  |

## Exposure Routes:

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| --- |
| inhalation, ingestion, skin and/or eye contactNIOSHDK2625000  |

## Symptoms:

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| --- |
| Eye irritation, conjunctivitis; keratitis (inflammation of the cornea); skin irritationNIOSHDK2625000  |

## Target Organs:

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| --- |
| Eyes, skinNIOSHDK2625000  |

## Incompatibility:

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| --- |
| Strong oxidizersNIOSHDK2625000  |

## Personal Protection:

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| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet or contaminated Change: Daily Provide: Eyewash, Quick drenchNIOSHDK2625000  |

## Exposure Limits:

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| --- |
| NIOSH REL : TWA 0. 4 mg/m 3 (0. 1 ppm) OSHA PEL : TWA 0. 4 mg/m 3 (0. 1 ppm)NIOSHDK2625000  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1026 (estimated with error: 57)NIST Spectramainlib\_227766, replib\_291109, replib\_1437, replib\_379808  |
| 905 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 180 C; CAS no: 106514; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb P AW DMCS; Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 912 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 190 C; CAS no: 106514; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb P AW DMCS; Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 919 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 200 C; CAS no: 106514; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb P AW DMCS; Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 923 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 210 C; CAS no: 106514; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb P AW DMCS; Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 1562 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 180 C; CAS no: 106514; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Chromosorb P AW DMCS (60-80 mesh); Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 1570 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 190 C; CAS no: 106514; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Chromosorb P AW DMCS (60-80 mesh); Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 1579 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 200 C; CAS no: 106514; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Chromosorb P AW DMCS (60-80 mesh); Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |
| 1587 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column length: 2 m; Column type: Packed; Start T: 210 C; CAS no: 106514; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Chromosorb P AW DMCS (60-80 mesh); Data type: Kovats RI; Authors: Llobera, A.; Garcia-Raso, A., Gas chromatographic behaviour of several p-quinones, J. Chromatogr., 393, 1987, 305-311.)NIST Spectranist ri  |

## Retention Index (Lee):

|  |
| --- |
| 143. 19 (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: 10 K/min; Start T: 40 C; End T: 310 C; Start time: 1 min; CAS no: 106514; Active phase: DB-5MS; Phase thickness: 0. 5 um; Data type: Lee RI; Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.; Roberts, D. W., Application of Lee retention indices to the confirmation of tentatively identified compounds from GC/MS analysis of environmental samples, Technical paper, Analytical Services Division, Environmental Science&Engineering, Inc, PO Box 1703, Gainesville, FL 32602, 2002, 11.)NIST Spectranist ri  |
| 147. 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: 4 K/min; Start T: 40 C; End T: 310 C; Start time: 1 min; CAS no: 106514; Active phase: DB-5MS; Phase thickness: 0. 5 um; Data type: Lee RI; Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.; Roberts, D. W., Application of Lee retention indices to the confirmation of tentatively identified compounds from GC/MS analysis of environmental samples, Technical paper, Analytical Services Division, Environmental Science&Engineering, Inc, PO Box 1703, Gainesville, FL 32602, 2002, 11.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 888 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 106514; Active phase: OV-101; Carrier gas: N2/He; Phase thickness: 0. 10 um; Data type: Normal alkane RI; Authors: Zenkevich, I. G., Experimentally measured retention indices., 2005.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 1. 3±0. 1 g/cm 3  |
| Boiling Point:  | 174. 0±15. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 1. 2±0. 3 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 41. 0±3. 0 kJ/mol  |
| Flash Point:  | 59. 3±17. 4 °C  |
| Index of Refraction:  | 1. 543  |
| Molar Refractivity:  | 27. 1±0. 3 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 0. 26  |
| ACD/LogD (pH 5. 5):  | 0. 13  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 28. 09  |
| ACD/LogD (pH 7. 4):  | 0. 13  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 28. 09  |
| Polar Surface Area:  | 34 Å 2  |
| Polarizability:  | 10. 8±0. 5 10 -24 cm 3  |
| Surface Tension:  | 47. 8±3. 0 dyne/cm  |
| Molar Volume:  | 86. 0±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. 25Log Kow (Exper. database match) = 0. 20Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 218. 08 (Adapted Stein & Brown method)Melting Pt (deg C): 23. 74 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0256 (Modified Grain method)MP (exp database): 115. 7 deg CVP (exp database): 9. 00E-02 mm Hg at 25 deg CSubcooled liquid VP: 0. 71 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): 7. 448e+004log Kow used: 0. 20 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1. 11e+004 mg/L (18 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 11100 mg/LWat Sol (Exper. database match) = 11100. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Quinone/HydroquinoneHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 22E-009 atm-m3/moleGroup Method: IncompleteExper Database: 4. 79E-05 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 889E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 20 (exp database)Log Kaw used: -2. 708 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 908Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7097Biowin2 (Non-Linear Model) : 0. 6382Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9153 (weeks )Biowin4 (Primary Survey Model) : 3. 6473 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6508Biowin6 (MITI Non-Linear Model): 0. 7660Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 2418Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 94. 7 Pa (0. 71 mm Hg)Log Koa (Koawin est ): 2. 908Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 17E-008 Octanol/air (Koa) model: 1. 99E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 14E-006 Mackay model : 2. 54E-006 Octanol/air (Koa) model: 1. 59E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 4. 5120 E-12 cm3/molecule-secHalf-Life = 2. 371 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 28. 447 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 350000 E-17 cm3/molecule-secHalf-Life = 3. 274 Days (at 7E11 mol/cm3)Half-Life = 78. 583 HrsFraction sorbed to airborne particulates (phi): 1. 84E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 387Log Koc: 0. 142 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. 20 (expkow database)Volatilization from Water: Henry LC: 4. 79E-005 atm-m3/mole (Henry experimental database)Half-Life from Model River: 13. 77 hoursHalf-Life from Model Lake : 237. 4 hours (9. 891 days)Removal In Wastewater Treatment: Total removal: 4. 33 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 72 percentTotal to Air: 2. 51 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 5. 5 32. 6 1000 Water 47. 4 360 1000 Soil 47 720 1000 Sediment 0. 088 3. 24e+003 0 Persistence Time: 281 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop