Benzoquinone c6h4o2 structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_6H_4O_2$
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113-115 °COxford University Chemical Safety Data (No longer updated)More details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)LabNetwork

LN00194634

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

°CLabNetworkLN0019463

4

- **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

  °CLabNetworkLN0019463

  4

- **Experimental Gravity:**

  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:**

  gold powderOxford University Chemical Safety Data (No longer updated)More details

  Pale-yellow solid with an acrid, chlorine-like odor. NIOSHDK2625000

- **Stability:**

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 Oxford University Chemical Safety Data (No longer updated)More details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  ORL-RAT LD50 100 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details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

  Eye: Irrigate immediately

  Skin: Soap wash

  immediately Breathing:

  Respiratory support

  Swallow: Medical

  attention

  immediatelyNIOSHDK262

  5000

- **Exposure Routes:**

  inhalation, ingestion, skin

  and/or eye

  contactNIOSHDK2625000

- **Symptoms:**

  Eye irritation,

  conjunctivitis; keratitis

  (inflammation of the

  cornea); skin

  irritationNIOSHDK2625000

- **Target Organs:**

  Eyes,

  skinNIOSHDK2625000

- **Incompatibility:**

  Strong

  oxidizersNIOSHDK2625000

- **Personal Protection:**

  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:**

  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: $10.8 \pm 0.5 \times 10^{-24}$ 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