Benzanthrone c17h10o structure

Contents

- Retention Index (Normal Alkane):

Molecular Formula	$C_{17}H_{10}O$
Average mass	230. 261 Da
Density	1. 3±0. 1 g/cm ^{3}
Boiling Point	436. 2±12. 0 °C at 760 mmHg
Flash Point	196. 1±14. 5 °C
Molar Refractivity	71. 8±0. 3 cm ^{3}
Polarizability	28. 5±0. 5 10^{-24} cm ^{3}
Surface Tension	58. 3±3. 0 dyne/cm
Molar Volume	178. 9±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule

- Experimental Physico-chemical Properties

  - **Experimental Melting Point:**

    176 °CTCIB0019

    171-175 °CAlfa Aesar

    170 °COxford University Chemical Safety Data (No longer updated)More details

    170 °CJean-Claude Bradley Open Melting Point Dataset15538, 21111

    173 °CJean-Claude Bradley Open Melting Point Dataset6222

    171-175 °CAlfa AesarB25322

  - **Experimental LogP:**

    4. 811Vitas-MSTK662686

  - **Experimental Flash Point:**

- Predicted Physico-chemical Properties

  - **Predicted Melting Point:**

    171-175 °CJ&K Scientific291143

    176 °CTCI

176 °CTCIB0019

- Miscellaneous

  - **Appearance:**

    light yellow powderOxford University Chemical Safety Data (No longer updated)More details

  - **Stability:**

    Stable. Incompatible with strong oxidizing agents. Oxford University Che Safety Data (No longer updated)More details

  - **Toxicity:**

    IPR-RAT LD50 1500 mg kg-1, IPR-MUS LD50 290 mg kg-1Oxford Universit Chemical Safety Data (No longer updated)More details

  - **Safety:**

    26-37Alfa AesarB25322

    26-37-60Alfa AesarB25322

    36/37/38Alfa AesarB25322

    H315-H319-H335Alfa AesarB25322

    P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarB25322

Safety glasses. Do not breathe dust. Oxford University Chemical Safety D

longer updated)More details

WarningAlfa AesarB25322

WARNING: Irreversible damage risk, protect skin/eyes/lungs. Alfa AesarB

XiAbblis ChemicalsAB1003202

- **Drug Status:**

  experimentalMicrosource[015

  05272]

- **Compound Source:**

  syntheticMicrosource[0150

  5272]

- Gas Chromatography

  - **Retention Index (Kovats):**

    2093 (estimated with error: 174)NIST Spectramainlib_231646, replib_109

    replib_261812, replib_155504

  - **Retention Index (Lee):**

    417. 7 (Program type: Ramp; Column cl... (show more)ass: Standard non

    Column type: Capillary; CAS no: 82053; Active phase: OV-101; Data type

    Authors: Tucminen, A.; Wickstrom, K.; Pyysalo, H., Determination of Polyc

    Aromatic Compounds by GLC-Selected Ion Monitoring (SIM) Technique, J.

Chromatogr. & Chromatogr. Comm., , 1986, 469-471.)NIST Spectranist ri

404. 39 (Program type: Ramp; Column cl… (show more)ass: Standard no
Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capilla
rate: 2 K/min; Start T: 120 C; End T: 280 C; CAS no: 82053; Active phase:
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: K
Balfanz, E.; Funcke, W.; Romanowski, T., Determination of oxygenated po
aromatic hydrocarbons in airborne particulate matter by capillary gas
chromatography and gas chromatography/mass spectrometry, Anal. Che
1983, 599-603.)NIST Spectranist ri

404. 4 (Program type: Ramp; Column cl… (show more)ass: Semi-standar
polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: C
CAS no: 82053; Active phase: DB-5MS; Data type: Lee RI; Authors: Aracil
R.; Conesa, J. A., Semivolatile and volatile compounds from the pyrolysis
combustion of polyvinyl chloride, J. Anal. Appl. Pyrolysis, 74, 2005, 465-4
Spectranist ri

405. 44 (Program type: Ramp; Column cl… (show more)ass: Semi-standa
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 6 K/min; Start T: 50 C; End T: 310 C; End time: 10 min; Start ti
min; CAS no: 82053; Active phase: HP-5; Carrier gas: Helium; Phase thick
25 um; Data type: Lee RI; Authors: Pedersen, D. U.; Durant, J. L.; Taghiza
Hemond, H. F.; Lafleur, A. L.; Cass, G. R., Human cell mutagenes in respi
airborne particles from the Northeastern United States. 2. Quantification
mutagenes and other organic compounds., Environ. Sci. Technol., 39(24)

9547-9560.)NIST Spectranist ri

404. 72 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Description: 60C(2min) => 15C/min => 180C => 5C/min => 2 (10min); CAS no: 82053; Active phase: LM-5; Carrier gas: He; Phase thick 25 um; Data type: Lee RI; Authors: Re-Poppi, N.; Santiago-Silva, M., Polyc aromatic hydrocarbons and other selected organic compounds in ambien Campo Grande City, Brazil, Atmos. Environ., 39, 2005, 2839-2850.)NIST Spectranist ri

403. 6 (Program type: Ramp; Column cl... (show more)ass: Semi-standar polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C CAS no: 82053; Active phase: DB-5; Phase thickness: 0. 25 um; Data type Authors: Lundstedt, S.; Haglund, P.; Oberg, L., Degradation and formation polycyclic aromatic compounds during bioslurry treatment of an aged ga soil, Environ. Toxicol. Chem., 22(7), 2003, 1413-1420.)NIST Spectranist r

404. 64 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Description: 60C(2min)=> 15C/min=> 180C=> 5C/min=> 280C(5min); CAS no: 82053; Active phase: LM-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Re-Poppi, N.; Santiago-S R., Identification of polycyclic aromatic hydrocarbons and methoxylated p in wood smoke emitted during production of charcoal, Chromatographia, 2002, 475-481.)NIST Spectranist ri

404. 85 (Program type: Isothermal; Col… (show more)umn class: Semi-st
non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; D
Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data
GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spe
ri

405 (Program type: Isothermal; Col… (show more)umn class: Semi-stand
polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data t
RI; Authors: Eckel, W. P., Making sense of nontarget compound data from
library searches, Am. Lab. Fairfield Conn., , 2000, 17-20., Program type:
Column cl… (show more)ass: Semi-standard non-polar; Column diameter
mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; St
C; End T: 300 C; Start time: 2 min; CAS no: 82053; Active phase: SPB-5;
type: Lee RI; Authors: Knobloch, T.; Engewald, W., Identification of some
polycyclic compounds in emissions from brown-coal-fired residential stov
Res. Chromatogr., 16, 1993, 239-242.)NIST Spectranist ri

405. 59 (Program type: Isothermal; Col… (show more)umn class: Semi-st
non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; D
Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data
GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spe
ri

409 (Program type: Isothermal; Col… (show more)umn class: Semi-stand
polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data t
RI; Authors: Eckel, W. P., Making sense of nontarget compound data from

library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spectranis

404. 9 (Program type: Ramp; Column cl... (show more)ass: Semi-standar
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 4 K/min; Start T: 40 C; End T: 300 C; Start time: 2 min; CAS no
Active phase: SPB-5; Data type: Lee RI; Authors: Knobloch, T.; Engewald,
Identification of some polar polycyclic compounds in emissions from brow
fired residential stoves, J. Hi. Res. Chromatogr., 16, 1993, 239-242.)NIST
Spectranist ri

407 (Program type: Complex; Column... (show more)class: Semi-standar
polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: C
Description: XX C ^ X C/min -> 170 C ^ 40 C/min -> 300 C (5 min); Chec
values XX and X (bad xerox copy); CAS no: 82053; Active phase: BP-5; D
Lee RI; Authors: Kelly, G. W.; Bartle, K. D.; Clifford, A. A.; Robinson, R. E.,
Application of coupled LC-GC to the analysis of the polar fraction of diese
particulate matter, J. Hi. Res. Chromatogr., 15, 1992, 526-530.)NIST Spec

- **Retention Index (Normal Alkane):**

2407 (Program type: Complex; Column... (show more)class: Standard no
Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capilla
Description: 50 0C (2 min) ^ 20 0C/min -> 160 0C ^ 5 0C/min -> 210 0C
0C/min -> 300 0C; CAS no: 82053; Active phase: Methyl Silicone; Carrier
Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Oda, J.
Yasuhara, A.; Matsunaga, K.; Saito, Y., Identification of polycyclic aromat
hydrocarbons of the particulate accumulated in the tunnel duct of freewa
generation of their oxygenated derivatives, Jpn. J. Toxicol. Environ. Healt

1998, 334-351.)NIST Spectranist ri

2428 (Program type: Complex; Column... (show more)class: Standard no

Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capilla

Description: 50 0C (2 min) ^ 20 0C/min -> 160 0C ^ 5 0C/min -> 210 0C

0C/min -> 300 0C; CAS no: 82053; Active phase: Methyl Silicone; Carrier

Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Oda, J.

Yasuhara, A.; Matsunaga, K.; Saito, Y., Identification of polycyclic aromat

hydrocarbons of the particulate accumulated in the tunnel duct of freewa

generation of their oxygenated derivatives, Jpn. J. Toxicol. Environ. Healt

1998, 334-351.)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:	436. 2±12. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±1. 0 mmHg at 25°C
Enthalpy of Vaporization:	69. 3±3. 0 kJ/mol
Flash Point:	196. 1±14. 5 °C
Index of Refraction:	1. 735
Molar Refractivity:	71. 8±0. 3 cm ^{3}
#H bond acceptors:	1

#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	4. 81
ACD/LogD (pH 5. 5):	4. 74
ACD/BCF (pH 5. 5):	2349. 56
ACD/KOC (pH 5. 5):	9006. 33
ACD/LogD (pH 7. 4):	4. 74
ACD/BCF (pH 7. 4):	2349. 56
ACD/KOC (pH 7. 4):	9006. 33
Polar Surface Area:	17 Å ^{2}
Polarizability:	28. 5±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	58. 3±3. 0 dyne/cm
Molar Volume:	178. 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) = 4. 73Log Kow (Exper. database match) = 4. 81Exper. Ref: Chem Inspect Test Inst (1992)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 403. 17 (Adapted Stein & Brown method)Melting Pt (deg C): 148. 49 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 21E-007 (Modified Grain method)MP (exp database): 170 deg CSubcooled liquid VP: 6. 96E-006 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): 0. 1837log Kow used: 4. 81 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 05221 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 61E-008 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 645E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 81 (exp database)Log Kaw used: -5. 568 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 10. 378Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6448Biowin2 (Non-Linear Model) : 0. 3287Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6678 (weeks-months)Biowin4 (Primary Survey Model) : 3. 4933 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2270Biowin6 (MITI Non-Linear Model): 0. 1104Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 5101Ready 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. 000928 Pa (6. 96E-006 mm Hg)Log Koa (Koawin est): 10. 378Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00323 Octanol/air (Koa) model: 0. 00586 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 105 Mackay model : 0. 205 Octanol/air (Koa) model: 0. 319 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 18. 0039 E-12 cm3/molecule-secHalf-Life = 0. 594 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 7. 129 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 155 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 221E+004Log Koc: 4. 087 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 = 2. 164 (BCF = 145. 8)log Kow used: 4. 81 (expkow database)Volatilization from Water: Henry LC: 6. 61E-008 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 344E+004 hours (560. 1 days)Half-Life from Model Lake : 1. 468E+005 hours (6116 days)Removal In Wastewater Treatment: Total removal: 70. 78 percentTotal biodegradation: 0. 63 percentTotal sludge adsorption: 70. 15 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. 214 14. 3 1000 Water 11. 1 900 1000 Soil 71. 9 1. 8e+003 1000 Sediment 16. 7 8. 1e+003 0 Persistence Time: 1. 62e+003 hr

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- 1-Click Docking
- 1-Click Scaffold Hop