

# [Benzanthrone c17h10o structure](https://assignbuster.com/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| 170 °COxford University Chemical Safety Data (No longer updated)More details |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:

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| --- |
| 4. 811Vitas-MSTK662686 |

## Experimental Flash Point:

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 171-175 °CJ&K Scientific291143 |
| 176 °CTCI |
| 176 °CTCIB0019 |

* Miscellaneous

## Appearance:

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| light yellow powderOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

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 Oxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

|  |
| --- |
| IPR-RAT LD50 1500 mg kg-1, IPR-MUS LD50 290 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |
| WarningAlfa AesarB25322 |
| WARNING: Irreversible damage risk, protect skin/eyes/lungs. Alfa AesarB25322 |
| XiAbblis ChemicalsAB1003202 |

## Drug Status:

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| experimentalMicrosource[01505272] |

## Compound Source:

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| --- |
| syntheticMicrosource[01505272] |

* Gas Chromatography

## Retention Index (Kovats):

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| 2093 (estimated with error: 174)NIST Spectramainlib\_231646, replib\_10998, replib\_261812, replib\_155504 |

## Retention Index (Lee):

|  |
| --- |
| 417. 7 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 82053; Active phase: OV-101; Data type: Lee RI; Authors: Tucminen, A.; Wickstrom, K.; Pyysalo, H., Determination of Polycyclic Aromatic Compounds by GLC-Selected Ion Monitoring (SIM) Technique, J. Hi. Res. Chromatogr. & Chromatogr. Comm., , 1986, 469-471.)NIST Spectranist ri |
| 404. 39 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 120 C; End T: 280 C; CAS no: 82053; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Konig, J.; Balfanz, E.; Funcke, W.; Romanowski, T., Determination of oxygenated polycyclic aromatic hydrocarbons in airborne particulate matter by capillary gas chromatography and gas chromatography/mass spectrometry, Anal. Chem., 55, 1983, 599-603.)NIST Spectranist ri |
| 404. 4 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; CAS no: 82053; Active phase: DB-5MS; Data type: Lee RI; Authors: Aracil, I.; Font, R.; Conesa, J. A., Semivolatile and volatile compounds from the pyrolysis and combustion of polyvinyl chloride, J. Anal. Appl. Pyrolysis, 74, 2005, 465-478.)NIST Spectranist ri |
| 405. 44 (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: 6 K/min; Start T: 50 C; End T: 310 C; End time: 10 min; Start time: 1. 5 min; CAS no: 82053; Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Pedersen, D. U.; Durant, J. L.; Taghizadeh, K.; Hemond, H. F.; Lafleur, A. L.; Cass, G. R., Human cell mutagenes in respirable airborne particles from the Northeastern United States. 2. Quantification of mutagenes and other organic compounds., Environ. Sci. Technol., 39(24), 2005, 9547-9560.)NIST Spectranist ri |
| 404. 72 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 60C(2min) => 15C/min => 180C => 5C/min => 280C (10min); CAS no: 82053; Active phase: LM-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Re-Poppi, N.; Santiago-Silva, M., Polycyclic aromatic hydrocarbons and other selected organic compounds in ambient air of Campo Grande City, Brazil, Atmos. Environ., 39, 2005, 2839-2850.)NIST Spectranist ri |
| 403. 6 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Lundstedt, S.; Haglund, P.; Oberg, L., Degradation and formation of polycyclic aromatic compounds during bioslurry treatment of an aged gasworks soil, Environ. Toxicol. Chem., 22(7), 2003, 1413-1420.)NIST Spectranist ri |
| 404. 64 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: 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-Silva, M. R., Identification of polycyclic aromatic hydrocarbons and methoxylated phenols in wood smoke emitted during production of charcoal, Chromatographia, 55(7/8), 2002, 475-481.)NIST Spectranist ri |
| 404. 85 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data type: Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data from GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spectranist ri |
| 405 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data type: Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data from GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20., 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: 300 C; Start time: 2 min; CAS no: 82053; Active phase: SPB-5; Data type: Lee RI; Authors: Knobloch, T.; Engewald, W., Identification of some polar polycyclic compounds in emissions from brown-coal-fired residential stoves, J. Hi. Res. Chromatogr., 16, 1993, 239-242.)NIST Spectranist ri |
| 405. 59 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data type: Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data from GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spectranist ri |
| 409 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; CAS no: 82053; Active phase: DB-5; Data type: Lee RI; Authors: Eckel, W. P., Making sense of nontarget compound data from GC-MS library searches, Am. Lab. Fairfield Conn., , 2000, 17-20.)NIST Spectranist ri |
| 404. 9 (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: 300 C; Start time: 2 min; CAS no: 82053; Active phase: SPB-5; Data type: Lee RI; Authors: Knobloch, T.; Engewald, W., Identification of some polar polycyclic compounds in emissions from brown-coal-fired residential stoves, J. Hi. Res. Chromatogr., 16, 1993, 239-242.)NIST Spectranist ri |
| 407 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Description: XX C ^ X C/min -> 170 C ^ 40 C/min -> 300 C (5 min); Check the values XX and X (bad xerox copy); CAS no: 82053; Active phase: BP-5; Data type: 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 diesel particulate matter, J. Hi. Res. Chromatogr., 15, 1992, 526-530.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

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| --- |
| 2407 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capillary; Description: 50 0C (2 min) ^ 20 0C/min -> 160 0C ^ 5 0C/min -> 210 0C ^ 10 0C/min -> 300 0C; CAS no: 82053; Active phase: Methyl Silicone; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Oda, J.; Yasuhara, A.; Matsunaga, K.; Saito, Y., Identification of polycyclic aromatic hydrocarbons of the particulate accumulated in the tunnel duct of freeway and generation of their oxygenated derivatives, Jpn. J. Toxicol. Environ. Health, 44(5), 1998, 334-351.)NIST Spectranist ri |
| 2428 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capillary; Description: 50 0C (2 min) ^ 20 0C/min -> 160 0C ^ 5 0C/min -> 210 0C ^ 10 0C/min -> 300 0C; CAS no: 82053; Active phase: Methyl Silicone; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Oda, J.; Yasuhara, A.; Matsunaga, K.; Saito, Y., Identification of polycyclic aromatic hydrocarbons of the particulate accumulated in the tunnel duct of freeway and generation of their oxygenated derivatives, Jpn. J. Toxicol. Environ. Health, 44(5), 1998, 334-351.)NIST Spectranist ri |

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

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| --- | --- |
| 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

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop