

# [Squalane c30h62 structure](https://assignbuster.com/squalane-c30h62-structure/)

Contents

* Retention Index (Linear):

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| --- | --- |
| Molecular Formula | C 30 H 62 |
| Average mass | 422. 813 Da |
| Density | 0. 8±0. 1 g/cm 3 |
| Boiling Point | 470. 3±0. 0 °C at 760 mmHg |
| Flash Point | 217. 8±0. 0 °C |
| Molar Refractivity | 140. 8±0. 3 cm 3 |
| Polarizability | 55. 8±0. 5 10 -24 cm 3 |
| Surface Tension | 28. 0±3. 0 dyne/cm |
| Molar Volume | 526. 0±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| -38 °CAlfa Aesar |
| -38 °COxford University Chemical Safety Data (No longer updated)More details |
| -38 °CJean-Claude Bradley Open Melting Point Dataset15187, 20416, 8422 |
| -38 °CAlfa AesarA17931 |
| -38 °C (Literature)LabNetworkLN00195308 |

## Experimental Boiling Point:

|  |
| --- |
| 210-215 deg C / 1 mm (500. 0104-507. 7479 °C / 760 mmHg)Alfa Aesar |
| 210-215 °COxford University Chemical Safety Data (No longer updated)More details |
| 210-215 °C / 1 mm (500. 0104-507. 7479 °C / 760 mmHg)Alfa AesarA17931 |

## Experimental Flash Point:

|  |
| --- |
| 218 °CAlfa Aesar |
| 217 °COxford University Chemical Safety Data (No longer updated)More details |
| 218 °CAlfa Aesar |
| 218 °F (103. 3333 °C)Alfa AesarA17931 |
| 424 °CLabNetworkLN00195308 |

## Experimental Gravity:

|  |
| --- |
| 20 g/mLMerck Millipore2544 |
| 20 g/lMerck Millipore2544, 814605 |
| 0. 81 g/mLAlfa AesarA17931 |

## Experimental Refraction Index:

|  |
| --- |
| 1. 451Alfa AesarA17931 |

* Miscellaneous

## Appearance:

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| --- |
| viscous colourless liquidOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

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 Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| 26-37Alfa AesarA17931 |
| 36/37/38Alfa AesarA17931 |
| GHS07BiosynthW-109407 |
| H315; H319; H335BiosynthW-109407 |
| H315-H319-H335Alfa AesarA17931 |
| P261; P305+P351+P338BiosynthW-109407 |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA17931 |
| Safety glasses. Oxford University Chemical Safety Data (No longer updated)More details |
| WarningAlfa AesarA17931 |
| WarningBiosynthW-109407 |
| WARNING: Irritates lungs, eyes, skinAlfa AesarA17931 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 2619 (estimated with error: 39)NIST Spectramainlib\_62218, replib\_17348, replib\_227596 |
| 2665 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 240 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 260 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2666 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 240 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 260 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2667 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 240 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2657 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 240 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2658. 1 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 260 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2658. 5 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 260 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Kovats RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

|  |
| --- |
| 2663 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Description: 50C=> 20C/min => 130C => 4C/min => 300C (20min); CAS no: 111013; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 2 um; Data type: Normal alkane RI; Authors: Kenig, F.; Sinninghe Damste, J. S.; Kock-van Dalen, A. C.; Rijpstra, W. I. C.; Huc, A. Y.; de Leeuw, J. W., Occurrence and origin of mono-, di-, and trimethylalkanes in modern and holocene cyanobacterial mats from Abu Dhabi, United Arab Emirates, Geochim. Cosmochim. Acta, 59(14), 1995, 2999-3015.)NIST Spectranist ri |
| 2668 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 21 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 40 C; End T: 280 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Normal alkane RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhideava, Capillary chromatography of polycyclic aromatic hydrocarbons on a home-produced capillary column with immobilized stationary liquid phase SE-30, Zh. Anal. Khim., 62(12), 1987, 2222-2226.)NIST Spectranist ri |
| 2657 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 240 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Normal alkane RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2658. 8 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Start T: 260 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Normal alkane RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2630 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 111013; Active phase: Apiezon; Data type: Normal alkane RI; Authors: Petrov, A. A., Hydrocarbons of petroleum, Nauka (publishing house), Moscow, 1984, 263., Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; Heat rate: 2 K/min; Start T: 130 C; End T: 300 C; CAS no: 111013; Active phase: Apiezon L; Data type: Normal alkane RI; Authors: Shlyakhov, A. F., Gas chromatography in organic geochemistry, Nedra, Moscow, 1984, 221.)NIST Spectranist ri |
| 2632 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 111013; Active phase: Apiezon; Data type: Normal alkane RI; Authors: Petrov, A. A., Hydrocarbons of petroleum, Nauka (publishing house), Moscow, 1984, 263.)NIST Spectranist ri |

## Retention Index (Linear):

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| 2664. 4 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 100 C; End T: 280 C; CAS no: 111013; Active phase: SE-30; Carrier gas: He; Data type: Linear RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |
| 2663 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 12. 5 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 120 C; End T: 325 C; End time: 5 min; CAS no: 111013; Active phase: Ultra-1; Carrier gas: He; Phase thickness: 0. 11 um; Data type: Linear RI; Authors: Tokuda, H.; Saitoh, E.; Kimura, Y.; Takano, S., Automated analysis of various compounds with a wide range of boiling points by capillary gas chromatgraphy based on retention indices, J. Chromatogr., 454, 1988, 109-120.)NIST Spectranist ri |
| 2660 (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: 50 C; End T: 260 C; Start time: 3 min; CAS no: 111013; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Zhao, Y. P.; Wang X. Y.; Wang, Z. C.; Lu Y.; Fu, C. X.; Chen, S. Y., Essential oil of Actinidia macrosperma, a catnip response kiwi endemic to China, Journal of Zhejiang University SCIENCE B, 7(9), 2006, 708-712.)NIST Spectranist ri |
| 2656. 1 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 21 mm; Column length: 17. 5 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 100 C; End T: 280 C; CAS no: 111013; Active phase: SE-52; Carrier gas: He; Data type: Linear RI; Authors: Pozhidaev, V. M.; Berezkin, V. G.; Korolev, A. A.; Popova, T. P.; Pozhidaeva, K. A., Retention indices of polycyclic aromatic hydrocarbons on quartz capillary columns with chemically immobilized stationary phases, Zh. Anal. Khim., 43, 1988, 1082-1088.)NIST Spectranist ri |

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

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| --- | --- |
| Density: | 0. 8±0. 1 g/cm 3 |
| Boiling Point: | 470. 3±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 5 mmHg at 25°C |
| Enthalpy of Vaporization: | 70. 5±0. 8 kJ/mol |
| Flash Point: | 217. 8±0. 0 °C |
| Index of Refraction: | 1. 448 |
| Molar Refractivity: | 140. 8±0. 3 cm 3 |
| #H bond acceptors: | 0 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 21 |
| #Rule of 5 Violations: | 1 |

|  |  |
| --- | --- |
| ACD/LogP: | 15. 59 |
| ACD/LogD (pH 5. 5): | 13. 46 |
| ACD/BCF (pH 5. 5): | 1000000. 00 |
| ACD/KOC (pH 5. 5): | 10000000. 00 |
| ACD/LogD (pH 7. 4): | 13. 46 |
| ACD/BCF (pH 7. 4): | 1000000. 00 |
| ACD/KOC (pH 7. 4): | 10000000. 00 |
| Polar Surface Area: | 0 Å 2 |
| Polarizability: | 55. 8±0. 5 10 -24 cm 3 |
| Surface Tension: | 28. 0±3. 0 dyne/cm |
| Molar Volume: | 526. 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) = 14. 63Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 408. 49 (Adapted Stein & Brown method)Melting Pt (deg C): 74. 73 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000275 (Modified Grain method)MP (exp database): -38 deg CBP (exp database): 350 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2. 042e-010log Kow used: 14. 63 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 4. 2283e-007 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 53E+003 atm-m3/moleGroup Method: 2. 03E+004 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 7. 493E+005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 14. 63 (KowWin est)Log Kaw used: 4. 796 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 834Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5462Biowin2 (Non-Linear Model) : 0. 0476Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2648 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2377 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 0559Biowin6 (MITI Non-Linear Model): 0. 0372Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3798Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 2. 5230BioHC Half-Life (days) : 333. 4541Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 0367 Pa (0. 000275 mm Hg)Log Koa (Koawin est ): 9. 834Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 18E-005 Octanol/air (Koa) model: 0. 00167 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 00295 Mackay model : 0. 0065 Octanol/air (Koa) model: 0. 118 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 40. 4595 E-12 cm3/molecule-secHalf-Life = 0. 264 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 172 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 00472 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 494E+008Log Koc: 8. 174 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: 14. 63 (estimated)Volatilization from Water: Henry LC: 1. 53E+003 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 2. 098 hoursHalf-Life from Model Lake : 195. 3 hours (8. 138 days)Removal In Wastewater Treatment: Total removal: 94. 04 percentTotal biodegradation: 0. 78 percentTotal sludge adsorption: 93. 25 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. 0902 6. 35 1000 Water 1. 9 900 1000 Soil 27. 9 1. 8e+003 1000 Sediment 70. 1 8. 1e+003 0 Persistence Time: 3. 1e+003 hr