

# [3-decyne c10h18 structure](https://assignbuster.com/3-decyne-c10h18-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 10 H 18  |
| Average mass  | 138. 250 Da  |
| Density  | 0. 8±0. 1 g/cm 3  |
| Boiling Point  | 179. 2±3. 0 °C at 760 mmHg  |
| Flash Point  | 52. 2±11. 2 °C  |
| Molar Refractivity  | 46. 4±0. 3 cm 3  |
| Polarizability  | 18. 4±0. 5 10 -24 cm 3  |
| Surface Tension  | 28. 3±3. 0 dyne/cm  |
| Molar Volume  | 176. 9±3. 0 cm 3  |

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

## Experimental Boiling Point:

|  |
| --- |
| 175-176 °CAlfa Aesar  |
| 175-176 °CAlfa AesarB20268  |

## Experimental Flash Point:

|  |
| --- |
| 56 °CAlfa Aesar  |
| 56 °CAlfa Aesar  |
| 56 °F (13. 3333 °C)Alfa AesarB20268  |

## Experimental Gravity:

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| --- |
| 0. 767 g/mLAlfa AesarB20268  |

## Experimental Refraction Index:

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| --- |
| 1. 435Alfa AesarB20268  |

* Miscellaneous

## Safety:

|  |
| --- |
| 3Alfa AesarB20268  |
| DANGER: FLAMMABLE, irritates skin and eyesAlfa AesarB20268  |
| H226Alfa AesarB20268  |
| P210-P280-P240-P303+P361+P353-P403+P235-P501aAlfa AesarB20268  |
| WarningAlfa AesarB20268  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1033 (estimated with error: 39)NIST Spectramainlib\_142633, replib\_114174, replib\_3520  |
| 1039 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 110 C; CAS no: 2384852; Active phase: OV-101; Carrier gas: He; Data type: Kovats RI; Authors: Kuningas, K.; Rang, S.; Kailas, T., Relationship between the structure and retention of n-alkenes and n-alkynes on silicone phases, J. Chromatogr., 520, 1990, 137-148.)NIST Spectranist ri  |
| 1014 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 100 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 90 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 107 m; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: H2; Phase thickness: 0. 40 um; Data type: Kovats RI; Authors: Sojak, L.; Farkas, P.; Ostrovsky, I.; Janak, J.; Chretien, J. R., Capillary gas chromatography of C5 – C13 branched alkynes on squalane and liquid crystal stationary phases, J. Chromatogr., 557, 1991, 241-253.)NIST Spectranist ri  |
| 1012 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 130 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460.)NIST Spectranist ri  |
| 1013 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 110 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 120 C; CAS no: 2384852; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460.)NIST Spectranist ri  |
| 1017 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 150 C; CAS no: 2384852; Active phase: Apiezon L; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460.)NIST Spectranist ri  |
| 1019 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 130 C; CAS no: 2384852; Active phase: Apiezon L; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460.)NIST Spectranist ri  |
| 1020 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 110 C; CAS no: 2384852; Active phase: Apiezon L; Carrier gas: N2; Data type: Kovats RI; Authors: Rang, S.; Kuningas, K.; Orav, A.; Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, J. Chromatogr., 119, 1976, 451-460.)NIST Spectranist ri  |
| 1190. 3 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: PEG-20M; Carrier gas: He; Phase thickness: 0. 13 um; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Kailas, T.; Koplimets, E.; Rang, S., Effect of adsorption on the retention values in capillary columns coated with OV-225 and PEG 20M, J. Chromatogr. A, 659, 1994, 143-150.)NIST Spectranist ri  |
| 1196. 2 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: PEG-20M; Carrier gas: He; Phase thickness: 0. 19 um; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Kailas, T.; Koplimets, E.; Rang, S., Effect of adsorption on the retention values in capillary columns coated with OV-225 and PEG 20M, J. Chromatogr. A, 659, 1994, 143-150.)NIST Spectranist ri  |
| 1199. 2 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: PEG-20M; Carrier gas: He; Phase thickness: 0. 22 um; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Kailas, T.; Koplimets, E.; Rang, S., Effect of adsorption on the retention values in capillary columns coated with OV-225 and PEG 20M, J. Chromatogr. A, 659, 1994, 143-150.)NIST Spectranist ri  |
| 1207 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 100 C; CAS no: 2384852; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 110 C; CAS no: 2384852; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 120 C; CAS no: 2384852; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 140 C; CAS no: 2384852; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri  |
| 1208 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: PEG 4000; Data type: Kovats RI; Authors: Rang, S. A.; Orav, A. E.; Kuningas, K. R.; Meister, A. E.; Strense, T. V.; Eisen, O. G., Gas-Chromatographic Characteristics of unsaturated hydrocarbons, Academy of Sciences of Estonia SSR, Tallinn, Estonia SSR, 1988, 208.)NIST Spectranist ri  |
| 1185. 3 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 61 C; CAS no: 2384852; Active phase: PEG-20M; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of n-tridecenes, n-tetradecenes and C10-C14 n-alkynes on polyethylene glycol 20m of different polarity, Eesti NSV Tead. Akad. Toim. Keem., 34(2), 1985, 105-113.)NIST Spectranist ri  |
| 1187. 5 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 70 C; CAS no: 2384852; Active phase: PEG-20M; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of n-tridecenes, n-tetradecenes and C10-C14 n-alkynes on polyethylene glycol 20m of different polarity, Eesti NSV Tead. Akad. Toim. Keem., 34(2), 1985, 105-113.)NIST Spectranist ri  |
| 1197. 5 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 61 C; CAS no: 2384852; Active phase: PEG-20M; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of n-tridecenes, n-tetradecenes and C10-C14 n-alkynes on polyethylene glycol 20m of different polarity, Eesti NSV Tead. Akad. Toim. Keem., 34(2), 1985, 105-113.)NIST Spectranist ri  |
| 1202. 7 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 70 C; CAS no: 2384852; Active phase: PEG-20M; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of n-tridecenes, n-tetradecenes and C10-C14 n-alkynes on polyethylene glycol 20m of different polarity, Eesti NSV Tead. Akad. Toim. Keem., 34(2), 1985, 105-113.)NIST Spectranist ri  |
| 1203. 1 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 80 C; CAS no: 2384852; Active phase: PEG-20M; Data type: Kovats RI; Authors: Orav, A.; Kuningas, K.; Rang, S.; Eisen, O., Capillary gas chromatography of n-tridecenes, n-tetradecenes and C10-C14 n-alkynes on polyethylene glycol 20m of different polarity, Eesti NSV Tead. Akad. Toim. Keem., 34(2), 1985, 105-113.)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:  | 179. 2±3. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 1. 3±0. 2 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 39. 8±0. 8 kJ/mol  |
| Flash Point:  | 52. 2±11. 2 °C  |
| Index of Refraction:  | 1. 437  |
| Molar Refractivity:  | 46. 4±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 6  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 4. 65  |
| ACD/LogD (pH 5. 5):  | 4. 45  |
| ACD/BCF (pH 5. 5):  | 1407. 19  |
| ACD/KOC (pH 5. 5):  | 6240. 06  |
| ACD/LogD (pH 7. 4):  | 4. 45  |
| ACD/BCF (pH 7. 4):  | 1407. 19  |
| ACD/KOC (pH 7. 4):  | 6240. 06  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 18. 4±0. 5 10 -24 cm 3  |
| Surface Tension:  | 28. 3±3. 0 dyne/cm  |
| Molar Volume:  | 176. 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. 54Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 179. 90 (Adapted Stein & Brown method)Melting Pt (deg C): 13. 39 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 52 (Mean VP of Antoine & Grain methods)BP (exp database): 177 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 3. 301log Kow used: 4. 54 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 9. 1072 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 89E-002 atm-m3/moleGroup Method: 7. 73E-002 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 8. 377E-002 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 54 (KowWin est)Log Kaw used: 0. 382 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 158Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7902Biowin2 (Non-Linear Model) : 0. 9473Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1920 (weeks )Biowin4 (Primary Survey Model) : 3. 9173 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5982Biowin6 (MITI Non-Linear Model): 0. 7596Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5152Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 6944BioHC Half-Life (days) : 4. 9477Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 185 Pa (1. 39 mm Hg)Log Koa (Koawin est ): 4. 158Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 62E-008 Octanol/air (Koa) model: 3. 53E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 85E-007 Mackay model : 1. 29E-006 Octanol/air (Koa) model: 2. 83E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 34. 8053 E-12 cm3/molecule-secHalf-Life = 0. 307 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 688 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 003000 E-17 cm3/molecule-secHalf-Life = 382. 000 Days (at 7E11 mol/cm3)Fraction sorbed to airborne particulates (phi): 9. 4E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1724Log Koc: 3. 236 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. 793 (BCF = 621. 6)log Kow used: 4. 54 (estimated)Volatilization from Water: Henry LC: 0. 0773 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 209 hoursHalf-Life from Model Lake : 111. 8 hours (4. 658 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 97. 67 percentTotal biodegradation: 0. 13 percentTotal sludge adsorption: 35. 99 percentTotal to Air: 61. 54 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 3 7. 37 1000 Water 22. 6 360 1000 Soil 65. 6 720 1000 Sediment 9. 46 3. 24e+003 0 Persistence Time: 270 hr

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