

# [Cetone c14h22o structure](https://assignbuster.com/cetone-c14h22o-structure/)

Contents

* Retention Index (Linear):

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| --- | --- |
| Molecular Formula | C 14 H 22 O |
| Average mass | 206. 324 Da |
| Density | 0. 9±0. 1 g/cm 3 |
| Boiling Point | 285. 3±29. 0 °C at 760 mmHg |
| Flash Point | 122. 1±17. 5 °C |
| Molar Refractivity | 66. 2±0. 3 cm 3 |
| Polarizability | 26. 2±0. 5 10 -24 cm 3 |
| Surface Tension | 32. 1±3. 0 dyne/cm |
| Molar Volume | 222. 0±3. 0 cm 3 |

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

## Experimental Boiling Point:

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| --- |
| 2 °C / 105 mmHg (55. 4141 °C / 760 mmHg)FooDBFDB008406, FDB008407 |

## Experimental Gravity:

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| --- |
| 0. 93 g/mLFluorochem |
| 0. 93 g/lFluorochem241698 |

* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 1506 (estimated with error: 57)NIST Spectramainlib\_196736, replib\_285401, replib\_108884 |
| 1471. 8 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 35 mm; Column length: 40 m; Column type: Capillary; Start T: 100 C; CAS no: 127515; Active phase: SE-30; Phase thickness: 0. 35 um; Data type: Kovats RI; Authors: Tudor, E., Temperature dependence of the retention index for perfumery compounds on a SE-30 glass capillary column. I. Linear equations, J. Chromatogr. A, 779, 1997, 287-297.)NIST Spectranist ri |
| 1877 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 127515; Active phase: Carbowax 20M; Phase thickness: 0. 45 um; Data type: Kovats RI; Authors: Tudor, E.; Moldovan, D.; Zarna, N., Temperature dependence of the retention index for perfumery compounds on two carbowax-20M glass capillary columns with different film thickness. 2, Rev. Roum. Chim., 44(7), 1999, 665-675.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

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| --- |
| 1476 (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: 3 K/min; Start T: 60 C; End T: 999 C; CAS no: 127515; Active phase: BPX-5; Carrier gas: Hydrogen; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Bieri, S.; Marriott, P. J., Dual-injection system with multiply injections for determining sidimentional retention indexes in comprehensive two-dimensional gas chromatography, Anal. Chem., 80, 2008, 760-768.)NIST Spectranist ri |
| 1481 (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: 3 K/min; Start T: 60 C; End T: 999 C; CAS no: 127515; Active phase: BPX-5; Carrier gas: Hydrogen; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Bieri, S.; Marriott, P. J., Dual-injection system with multiply injections for determining sidimentional retention indexes in comprehensive two-dimensional gas chromatography, Anal. Chem., 80, 2008, 760-768.)NIST Spectranist ri |
| 1482 (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: 3 K/min; Start T: 60 C; End T: 999 C; CAS no: 127515; Active phase: BPX-5; Carrier gas: Hydrogen; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Bieri, S.; Marriott, P. J., Dual-injection system with multiply injections for determining sidimentional retention indexes in comprehensive two-dimensional gas chromatography, Anal. Chem., 80, 2008, 760-768.)NIST Spectranist ri |
| 1484 (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: 3 K/min; Start T: 100 C; End T: 999 C; CAS no: 127515; Active phase: BPX-5; Carrier gas: Hydrogen; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Bieri, S.; Marriott, P. J., Dual-injection system with multiply injections for determining sidimentional retention indexes in comprehensive two-dimensional gas chromatography, Anal. Chem., 80, 2008, 760-768.)NIST Spectranist ri |
| 1486 (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: 5 K/min; Start T: 60 C; End T: 999 C; CAS no: 127515; Active phase: BPX-5; Carrier gas: Hydrogen; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Bieri, S.; Marriott, P. J., Dual-injection system with multiply injections for determining sidimentional retention indexes in comprehensive two-dimensional gas chromatography, Anal. Chem., 80, 2008, 760-768.)NIST Spectranist ri |
| 1473 (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: 1. 5 K/min; Start T: 40 C; End T: 260 C; CAS no: 127515; Active phase: Equity-5 MS; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mondello, L.; Casilli, A.; Tranchida, Q.; Sciarrone, D.; Dugo, P.; Dugo, G., Analysis of allergens in fragrances using multiple heart-cut multidimentional gas chromatography – mass spectrometry, LC-GC Europe, 21, 2008, 130.)NIST Spectranist ri |
| 1471 (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: 127515; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparation and identification of volatile compounds in Changyu XO brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri |
| 1508 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C (2 min) ^ 5 0C/min -> 80 0C ^ 7 oC/min -> 160 0C ^ 9 0C/min -> 200 0C ^ 20 0C/min -> 280 0C (10 min); CAS no: 127515; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparation and identification of volatile compounds in Changyu XO brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri |
| 1479 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column type: Capillary; Description: 50C => 3C/min => 200C(10min) => 10C/min => 290C(10min); CAS no: 127515; Active phase: HP-5; Carrier gas: He; Data type: Normal alkane RI; Authors: Splivallo, R.; Bossi, S.; Maffei, M.; Bonfante, P., Discrimination of truffle fruiting body versus mycelial aromas by stir bar sorptive extraction, Phytochemistry, 68, 2007, 2584-2598.)NIST Spectranist ri |
| 1484. 5 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 260 C; End time: 28 min; Start time: 2 min; CAS no: 127515; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Leffingwell, J. C.; Alford, E. D., Volatile constituents of Perique tobacco, Electron. J. Environ. Agric. Food Chem., 4(2), 2005, 899-915.)NIST Spectranist ri |
| 1848 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Description: 40C(3min) => 10C/min => 90C => 2C/min => 230C (37min); CAS no: 127515; Active phase: DB-Wax Etr; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Loskos, N.; Hernandez-Orte, P.; Cacho, J.; Ferreira, V., Release and formation of varietal aroma compounds during alcoholic fermentation from nonfloral grape odorless flavor precursors fractions, J. Agric. Food Chem., 55, 2007, 6674-6684.)NIST Spectranist ri |

## Retention Index (Linear):

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| 1478 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 250 C; CAS no: 127515; Active phase: SE-30; Data type: Linear RI; Authors: Paramonov, E. A.; Khalilova, A. Z.; Odinokov, V. N.; Khalilov, L. M., Identification and biological activity of volatile organic compounds isolated from plants and insects. III. Chromatography-mass spectrometry of volatile compoundsof Aegopodium podagraria, Chem. Nat. Compd. (Engl. Transl.), 36(6), 2000, 584-586, In original 466-467.)NIST Spectranist ri |
| 1490 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 26 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 100 C; End T: 250 C; CAS no: 127515; Active phase: CP Sil 5 CB; Phase thickness: 1. 25 um; Data type: Linear RI; Authors: Halket, J. M.; Schulten, H.-R., Thick-film capillary column gas chromatography-field ionization mass spectrometry: A complementary technique for the rapid analysis of volatiles, J. Chromatogr., 322, 1985, 200-205.)NIST Spectranist ri |
| 1494 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 26 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 100 C; End T: 250 C; CAS no: 127515; Active phase: CP Sil 5 CB; Phase thickness: 1. 25 um; Data type: Linear RI; Authors: Halket, J. M.; Schulten, H.-R., Thick-film capillary column gas chromatography-field ionization mass spectrometry: A complementary technique for the rapid analysis of volatiles, J. Chromatogr., 322, 1985, 200-205.)NIST Spectranist ri |
| 1473 (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: 127515; Active phase: SLB-5MS; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Mondello, L.; Sciarrone, D.; Casilli, A.; Tranchida, P. Q.; Dugo, P.; Dugo, G., Fast gas chromatography-full scan quadrupole mass spectrometry for the determination of allergens in fragrances, J. Sep. Sci., 30, 2007, 1905-1911., Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; Heat rate: 7 K/min; Start T: 50 C; End T: 325 C; End time: 10 min; CAS no: 127515; Active phase: SLB-5ms; Data type: Linear RI; Authors: Mondello, L.; Costa, R., A new generation of GC capillary columns: SLB-5ms, The Reporter (Europe), 20(March), 2006, 17-19.)NIST Spectranist ri |
| 1480 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 1 mm; Column length: 10 m; Column type: Capillary; Heat rate: 40 K/min; Start T: 40 C; End T: 250 C; CAS no: 127515; Active phase: SLB-5MS; Phase thickness: 0. 1 um; Data type: Linear RI; Authors: Mondello, L.; Sciarrone, D.; Casilli, A.; Tranchida, P. Q.; Dugo, P.; Dugo, G., Fast gas chromatography-full scan quadrupole mass spectrometry for the determination of allergens in fragrances, J. Sep. Sci., 30, 2007, 1905-1911.)NIST Spectranist ri |
| 1481 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 1 mm; Column length: 10 m; Column type: Capillary; Heat rate: 40 K/min; Start T: 40 C; End T: 250 C; CAS no: 127515; Active phase: SLB-5MS; Phase thickness: 0. 1 um; Data type: Linear RI; Authors: Mondello, L.; Sciarrone, D.; Casilli, A.; Tranchida, P. Q.; Dugo, P.; Dugo, G., Fast gas chromatography-full scan quadrupole mass spectrometry for the determination of allergens in fragrances, J. Sep. Sci., 30, 2007, 1905-1911.)NIST Spectranist ri |
| 1470 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; Heat rate: 7 K/min; Start T: 50 C; End T: 325 C; End time: 10 min; CAS no: 127515; Active phase: 5 % Phenyl methyl siloxane; Data type: Linear RI; Authors: Mondello, L.; Costa, R., A new generation of GC capillary columns: SLB-5ms, The Reporter (Europe), 20(March), 2006, 17-19.)NIST Spectranist ri |
| 1474 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; Heat rate: 7 K/min; Start T: 50 C; End T: 325 C; End time: 10 min; CAS no: 127515; Active phase: SLB-5ms; Data type: Linear RI; Authors: Mondello, L.; Costa, R., A new generation of GC capillary columns: SLB-5ms, The Reporter (Europe), 20(March), 2006, 17-19.)NIST Spectranist ri |

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

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| --- | --- |
| Density: | 0. 9±0. 1 g/cm 3 |
| Boiling Point: | 285. 3±29. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 6 mmHg at 25°C |
| Enthalpy of Vaporization: | 52. 4±3. 0 kJ/mol |
| Flash Point: | 122. 1±17. 5 °C |
| Index of Refraction: | 1. 508 |
| Molar Refractivity: | 66. 2±0. 3 cm 3 |
| #H bond acceptors: | 1 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 2 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 4. 41 |
| ACD/LogD (pH 5. 5): | 4. 22 |
| ACD/BCF (pH 5. 5): | 947. 63 |
| ACD/KOC (pH 5. 5): | 4701. 95 |
| ACD/LogD (pH 7. 4): | 4. 22 |
| ACD/BCF (pH 7. 4): | 947. 63 |
| ACD/KOC (pH 7. 4): | 4701. 95 |
| Polar Surface Area: | 17 Å 2 |
| Polarizability: | 26. 2±0. 5 10 -24 cm 3 |
| Surface Tension: | 32. 1±3. 0 dyne/cm |
| Molar Volume: | 222. 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) = 4. 84Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 271. 60 (Adapted Stein & Brown method)Melting Pt (deg C): 45. 26 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00972 (Modified Grain method)Subcooled liquid VP: 0. 0149 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): 2. 98log Kow used: 4. 84 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 6. 9473 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Vinyl/Allyl KetonesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 83E-004 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 8. 855E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 84 (KowWin est)Log Kaw used: -1. 937 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 777Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 4722Biowin2 (Non-Linear Model) : 0. 1094Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5086 (weeks-months)Biowin4 (Primary Survey Model) : 3. 3744 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3500Biowin6 (MITI Non-Linear Model): 0. 1544Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 6355Ready 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): 1. 99 Pa (0. 0149 mm Hg)Log Koa (Koawin est ): 6. 777Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 51E-006 Octanol/air (Koa) model: 1. 47E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 45E-005 Mackay model : 0. 000121 Octanol/air (Koa) model: 0. 000118 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 170. 7666 E-12 cm3/molecule-secHalf-Life = 0. 063 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 752 HrsOzone Reaction: OVERALL Ozone Rate Constant = 62. 963127 E-17 cm3/molecule-secHalf-Life = 0. 018 Days (at 7E11 mol/cm3)Half-Life = 26. 210 MinReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 8. 77E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1034Log Koc: 3. 014 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 = 3. 028 (BCF = 1066)log Kow used: 4. 84 (estimated)Volatilization from Water: Henry LC: 0. 000283 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 4. 437 hoursHalf-Life from Model Lake : 168. 9 hours (7. 036 days)Removal In Wastewater Treatment: Total removal: 73. 43 percentTotal biodegradation: 0. 61 percentTotal sludge adsorption: 69. 87 percentTotal to Air: 2. 95 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0201 0. 338 1000 Water 9. 15 900 1000 Soil 76. 1 1. 8e+003 1000 Sediment 14. 7 8. 1e+003 0 Persistence Time: 1. 13e+003 hr

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