

Cetone c14h22o structure



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Contents

- Retention Index (Linear):

Molecular Formula	$C_{14}H_{22}O$
Average mass	206.324 Da
Density	$0.9 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$285.3 \pm 29.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$122.1 \pm 17.5 \text{ }^\circ\text{C}$
Molar Refractivity	$66.2 \pm 0.3 \text{ cm}^3$
Polarizability	$26.2 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	32.1 ± 3.0 dyne/cm
Molar Volume	$222.0 \pm 3.0 \text{ cm}^3$

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

- **Experimental Boiling Point:**

2 °C / 105 mmHg

(55. 4141 °C / 760

mmHg)FooDBFDB

008406,

FDB008407

- **Experimental Gravity:**

0. 93 g/mLFluorochem

0. 93

g/lFluorochem241698

- Gas Chromatography

- **Retention Index (Kovats):**

1506 (estimated

with error:

57)NIST

Spectramainlib_19

6736,

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):**

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
multiple injections
for determining
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
sidimensional
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
multiple injections
for determining
two-dimensional
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
sidimensional
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
sidimensional
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
multidimensional
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 0C/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):**

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 μm ; 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 μ m; 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

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

<https://assignbuster.com/cetone-c14h22o-structure/>

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

[Click to predict properties on the Chemicalize site](https://assignbuster.com/cetone-c14h22o-structure/)