

2-acetoxy-3-butanone
c6h10o3 structure



**ASSIGN
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\n[[toc title="Table of Contents"](#)]\n

\n \t

1. [Experimental Boiling Point:](#) \n \t
2. [Experimental Flash Point:](#) \n \t
3. [Experimental Gravity:](#) \n \t
4. [Experimental Refraction Index:](#) \n \t
5. [Appearance:](#) \n \t
6. [Safety:](#) \n \t
7. [Retention Index \(Kovats\):](#) \n \t
8. [Retention Index \(Normal Alkane\):](#) \n \t
9. [Retention Index \(Linear\):](#) \n

\n[/toc]\n \n

Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_{10}O_3$
Average mass	130. 142 Da
Density	$1. 0 \pm 0. 1 \text{ g/cm}^3$
Boiling Point	$163. 4 \pm 23. 0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$56. 6 \pm 22. 7 \text{ }^\circ\text{C}$

<https://assignbuster.com/2-acetoxy-3-butanone-c6h10o3-structure/>

Molar
Refractivity $31.6 \pm 0.3 \text{ cm}^3$

Polarizability $12.5 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface 28.9 ± 3.0

Tension dyne/cm

Molar $128.6 \pm 3.0 \text{ cm}^3$

Volume 3

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

- **Experimental Boiling Point:**

154-155 °C Alfa

Aesar

74-75 °C / 20 mm

Hg (193.7316-

195.0446 °C / 760

mmHg) Food and

Agriculture
Organization of
the United
Nations1-Methyl-
2-oxopropyl
acetate

154-155 °CAlfa
AesarL06927

169-173
°CFooDBFDB0118
08

- **Experimental Flash Point:**

66 °CAlfa Aesar

66 °CAlfa Aesar

66 °F (18. 8889

°C)Alfa

AesarL06927

- **Experimental Gravity:**

1. 025 g/mLAlfa

AesarL06927

- **Experimental Refraction Index:**

1. 412Alfa

AesarL06927

1. 41-1. 416Food

and Agriculture

Organization of

the United

Nations1-Methyl-

2-oxopropyl

acetate

- Miscellaneous

- **Appearance:**

colourless to

slightly yellow

liquidFood and

Agriculture

Organization of

the United

Nations1-Methyl-

2-oxopropyl

acetate

- **Safety:**

23-26-37Alfa

AesarL06927

36/38Alfa

AesarL06927

H315-H319Alfa

AesarL06927

IRRITANTAlfa

AesarL06927

P280-

P305+P351+P338

-P362-P321-

P332+P313-

P337+P313Alfa

AesarL06927

WarningAlfa

AesarL06927

WARNING: Irritates

skin and eyesAlfa

AesarL06927

- Gas Chromatography

- **Retention Index (Kovats):**

857 (estimated)

with error: 89)NIST

Spectramainlib_35

2267

- **Retention Index (Normal Alkane):**

857 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard non-

polar; Column

diameter: 0. 32

mm; Column

length: 50 m;

Column type:

Capillary; Heat

rate: 5 K/min;

Start T: 65 C; End

T: 280 C; End

time: 30 min; Start

time: 10 min; CAS

no: 4906245;

Active phase: CP

Sil 5 CB; Carrier

gas: He; Phase

thickness: 0. 4

um; Data type:
Normal alkane RI;
Authors: Joulain,
D.; Casazza, A.;
Laurent, R.;
Portier, D.;
Guillamon, N.;
Pandya, R.; Le, M.;
Viljoen, A., Volatile
flavor constituents
of fruits from
Southern Africa:
mobola plum
(Parinari
curatellifolia), J.
Agric. Food Chem.,
52, 2004, 2322-
2325.)NIST
Spectranist ri

852 (Program
type: Ramp;
Column cl... (show
more)ass:
Standard non-
polar; Column

diameter: 0. 25
mm; Column
length: 30 m;
Column type:
Capillary; Heat
rate: 5 K/min;
Start T: 50 C; End
T: 240 C; Start
time: 3 min; CAS
no: 4906245;
Active phase: DB-
1; Carrier gas: He;
Phase thickness:
0. 25 um; Data
type: Normal
alkane RI; Authors:
Shiota, H., New
esteric
components in the
volatiles of banana
fruit (Musa
sapiantum L.), J.
Agric. Food Chem.,
41(11), 1993,
2056-2062.)NIST

Spectranist ri

856 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard non-

polar; Column

diameter: 0. 25

mm; Column

length: 30 m;

Column type:

Capillary; Heat

rate: 5 K/min;

Start T: 50 C; End

T: 240 C; Start

time: 3 min; CAS

no: 4906245;

Active phase: DB-

1; Carrier gas: He;

Phase thickness:

0. 25 um; Data

type: Normal

alkane RI; Authors:

Shiota, H., New

esteric

components in the
volatiles of banana

fruit (Musa

sapientum L.), J.

Agric. Food Chem.,

41(11), 1993,

2056-2062.,

Program type:

Ramp; Column

cl... (show

more)ass:

Standard non-

polar; Column

diameter: 0. 25

mm; Column

length: 60 m;

Column type:

Capillary; Heat

rate: 3 K/min;

Start T: 50 C; End

T: 240 C; CAS no:

4906245; Active

phase: DB-1;

Carrier gas: He;

Phase thickness:

0. 25 um; Data

type: Normal
alkane RI; Authors:
Shiota, H., Volatile
components of
pawpaw fruit
(Asimina triloba
Dunal.), J. Agric.
Food Chem.,
39(9), 1991, 1631-
1635.)NIST
Spectranist ri

855 (Program
type: Ramp;
Column cl... (show
more)ass:
Standard non-
polar; Column
diameter: 0. 25
mm; Column
length: 60 m;
Column type:
Capillary; Heat
rate: 3 K/min;
Start T: 50 C; End
T: 240 C; CAS no:

4906245; Active

phase: DB-1;

Carrier gas: He;

Phase thickness:

0. 25 um; Data

type: Normal

alkane RI; Authors:

Shiota, H., Volatile

components of

pawpaw fruit

(Asimina triloba

Dunal.), J. Agric.

Food Chem.,

39(9), 1991, 1631-

1635.)NIST

Spectranist ri

1378 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard polar;

Column diameter:

0. 25 mm; Column

length: 60 m;

Column type:

Capillary; Heat
rate: 3 K/min;
Start T: 40 C; End
T: 220 C; End
time: 10 min; Start
time: 10 min; CAS
no: 4906245;
Active phase: DB-
Wax; Carrier gas:
He; Phase
thickness: 0. 25
um; Data type:
Normal alkane RI;
Authors: Hayata,
Y.; Sakamoto, T.;
Kozuka, H.;
Sakamoto, K.;
Osajima, Y.,
Analysis of
aromatic volatile
compounds in '
Miyabi' melon
(Cucumis melo L.)
using the Porapak
Q column, J. Jpn.
Soc. Hortic. Sci.,

71(4), 2002, 517-

525.)NIST

Spectranist ri

- **Retention Index (Linear):**

1389 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard polar;

Column diameter:

0.25 mm; Column

length: 30 m;

Column type:

Capillary; Heat

rate: 5 K/min;

Start T: 40 C; End

T: 250 C; End

time: 15 min; Start

time: 3 min; CAS

no: 4906245;

Active phase: DB-

Wax Etr; Carrier

gas: He; Phase

thickness: 0.25

um; Data type:

Linear RI; Authors:
Aubert C.; Pitrat
M., Volatile
compounds in the
skin and pulp of
Queen Anne's
pocket melon, J.
Agric. Food Chem.,
54, 2006, 8177-
8182., Program
type: Ramp;
Column cl... (show
more)ass:
Standard polar;
Column diameter:
0.32 mm; Column
length: 30 m;
Column type:
Capillary; Heat
rate: 5 K/min;
Start T: 40 C; End
T: 240 C; Start
time: 2 min; CAS
no: 4906245;
Active phase: DB-
FFAP; Carrier gas:

H2; Phase

thickness: 0.25

um; Data type:

Linear RI; Authors:

Charles, M.;

Martin, B.; Ginies,

C.; Etievant, P.;

Coste, G.;

Guichard, E.,

Potent aroma

compounds of two

red wine vinegars,

J. Agric. Food

Chem., 48, 2000,

70-77.)NIST

Spectranist ri

1377 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard polar;

Column diameter:

0.25 mm; Column

length: 30 m;

Column type:

Capillary; Heat
rate: 2 K/min;
Start T: 40 C; End
T: 200 C; Start
time: 10 min; CAS
no: 4906245;
Active phase: DB-
Wax; Carrier gas:
He; Data type:
Linear RI; Authors:
Umano, K.; Hagi,
Y.; Nakahara, K.;
Shoji, A.;
Shibamoto, T.,
Volatile
constituents of
green and ripened
pineapple (*Ananas
comosus* [L.]
Merr.), *J. Agric.
Food Chem.*,
40(4), 1992, 599-
603.)NIST
Spectranist ri
1358 (Program

type: Ramp;
Column cl... (show
more)ass:
Standard polar;
Column diameter:
0. 25 mm; Column
length: 30 m;
Column type:
Capillary; Heat
rate: 4 K/min;
Start T: 50 C; End
T: 250 C; Start
time: 3 min; CAS
no: 4906245;
Active phase: DB-
Wax; Carrier gas:
He; Phase
thickness: 0. 25
um; Data type:
Linear RI; Authors:
Frohlich, O.;
Duque, C.;
Schreier, P.,
Volatile
constituents of
curuba (Passiflora

mollissima) fruit, J.

Agric. Food Chem.,

37(2), 1989, 421-

425.)NIST

Spectranist ri

1361 (Program

type: Ramp;

Column cl... (show

more)ass:

Standard polar;

Column diameter:

0. 25 mm; Column

length: 30 m;

Column type:

Capillary; Heat

rate: 4 K/min;

Start T: 50 C; End

T: 250 C; Start

time: 3 min; CAS

no: 4906245;

Active phase: DB-

Wax; Carrier gas:

He; Phase

thickness: 0. 25

um; Data type:

Linear RI; Authors:

Frohlich, O.;

Duque, C.;

Schreier, P.,

Volatile

constituents of

curuba (Passiflora

mollissima) fruit, J.

Agric. Food Chem.,

37(2), 1989, 421-

425.)NIST

Spectranist ri

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

Density:	1. 0±0. 1 g/cm ³
Boiling Point:	163. 4±23. 0 °C at 760 mmHg
Vapour Pressure:	2. 1±0. 3 mmHg at 25°C
Enthalpy of Vaporization:	40. 0±3. 0 kJ/mol
Flash Point:	56. 6±22. 7 °C
Index of Refraction:	1. 406
Molar Refractivity:	31. 6±0. 3 cm ³

#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	0.68
ACD/LogD (pH 5.5):	0.26
ACD/BCF (pH 5.5):	1.00
ACD/KOC (pH 5.5):	33.10
ACD/LogD (pH 7.4):	0.26
ACD/BCF (pH 7.4):	1.00
ACD/KOC (pH 7.4):	33.10
Polar Surface Area:	43 Å ²
Polarizability:	12.5 ± 0.5 10 ⁻²⁴ cm ³
Surface Tension:	28.9 ± 3.0 dyne/cm
Molar Volume:	128.6 ± 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) = 0. 22 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 156. 08 (Adapted Stein & Brown method) Melting Pt (deg C): -30. 52 (Mean or Weighted MP) VP (mm Hg, 25 deg C): 3. 02 (Mean VP of Antoine & Grain methods) Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 5. 921e+004 log Kow used: 0. 22 (estimated) no-melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3. 1895e+005 mg/L ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Esters Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 11E-006 atm-m³/mole Group Method: Incomplete Henrys LC [VP/WSol estimate using EPI values]: 8. 734E-006 atm-m³/mole Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 22 (KowWin est) Log Kaw used: -4. 343 (HenryWin est) Log Koa (KOAWIN v1. 10 estimate): 4. 563 Log Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8666 Biowin2 (Non-Linear Model) : 0. 9917 Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0293 (weeks) Biowin4 (Primary Survey Model) : 3. 8667 (days) MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7370 Biowin6 (MITI Non-Linear Model): 0. 8815 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2115 Ready Biodegradability Prediction: YES Hydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 367 Pa (2. 75 mm Hg) Log Koa (Koawin est) : 4. 563 Kp (particle/gas partition coef. (m³/ug)): Mackay model : 8. 18E-009 Octanol/air (Koa) model: 8. 97E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 96E-007 Mackay model : 6. 55E-007 Octanol/air (Koa) model: 7. 18E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 3. 0026 E-12 cm³/mole-sec Half-Life = 3. 562 Days (12-hr day; 1. 5E6 OH/cm³) Half-Life = 42. 747 Hrs Ozone Reaction: No Ozone Reaction Estimation Fraction sorbed to airborne particulates (phi): 4. 75E-007 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 634 Log Koc: 0. 213 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 9. 082E-002 L/mol-sec Kb Half-Life at pH 8: 88. 325 days Kb Half-Life at pH 7: 2. 418 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 500 (BCF = 3. 162) log Kow used: 0. 22 (estimated) Volatilization from Water: Henry LC: 1. 11E-006 atm-m³/mole (estimated by Bond SAR Method) Half-Life from Model River: 602. 9 hours (25. 12 days) Half-Life from Model Lake : 6673 hours (278 days) Removal In Wastewater Treatment: Total removal: 1. 92 percent Total biodegradation: 0. 09 percent Total sludge adsorption: 1. 76 percent Total to Air: 0. 06 percent (using 10000 hr Bio P, A, S) Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 4. 58 85. 5 1000 Water 44. 5 360 1000 Soil 50. 8 720 1000 Sediment 0. 0828 3. 24e+003 0 Persistence Time: 382 hr

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