Ethyl linoleate (jan) c20h36o2 structure

\n[toc title="Table of Contents"]\n

\n \t

\n[/toc]\n \n

Contents

Molecular Formula	$C_{20}H_{36}O_2$
Average mass	308. 499 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	388. 3±21. 0 °C at 760 mmHg
Flash Point	96. 3±20. 4 °C
Molar Refractivity	96. 6±0. 3 cm ^{3}
Polarizability	38. 3±0. 5 10^{-24} cm ^{3}
Surface Tension	31. 4±3. 0 dyne/cm

Molar Volume 349. 4±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Gas Chromatography

Retention Index (Kovats):

2193 (estimated with error: 47)NIST Spectramainlib_155747, replib_229299, replib_55769

Retention Index (Normal Alkane):

2159 (Program type: Ramp; Column cl... (show more)ass: Standard non-p
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 5 K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start time: 5
CAS no: 544354; Active phase: SE-30; Carrier gas: He; Phase thickness: 0
Data type: Normal alkane RI; Authors: Loizzo, M. R.; Tundis, R.; Conforti,
A. M.; Statti, G. A.; Menichini, F., Comparative chemical composition, anti
and hypoglycaemic activities of Juniperus oxycedrus ssp. oxycedrus L. be
wood oils from Lebanon, Food Chem., 105, 2007, 572-578.)NIST Spectran

2140 (Program type: Ramp; Column cl... (show more)ass: Standard non-p
Column type: Capillary; CAS no: 544354; Active phase: SE-30; Data type:
alkane RI; Authors: Vinogradov, B. A., Production, composition, properties
application of essential oils, 2004.)NIST Spectranist ri

2162 (Program type: Complex; Column... (show more)class: Semi-standa
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Description: 35C=> 5C/min => 160C=> 10C/min => 220C (10min); CAS
544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 u
type: Normal alkane RI; Authors: Demyttenaere, J. C. R.; Sanchez Martine
Tellez Valdes, M. J.; Verhe, R.; Sandra, P., Analysis of volatile esters of ma
whisky using solid phase microextraction and dynamic headspace, in 25t
International Symposium on Capillary Chromatography, 2002, 1-13., Prog
type: Complex; Column... (show more)class: Semi-standard non-polar; Co
diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Descr
35C=> 5C/min=> 220C=> 10C/min=> 240C(5min); CAS no: 544354; Ac
phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Norm
alkane RI; Authors: Demyttenaere, J. C. R.; Sanchez Martinez, J. I.; Verhe,
Sandra, P.; de Kimpe, N., Analysis of volatiles of malt whisky by solid-pha
microextraction and stir bar sorptive extraction, J. Chromatogr. A, 985, 2
221-232., Program type: Complex; Column... (show more)class: Standard
polar; Column diameter: 0. 28 mm; Column length: 40 m; Column type: C
Description: 75C => 3C/min => 190C(25min) => 3C/min => 210C; CAS
544354; Active phase: SF-96; Data type: Normal alkane RI; Authors: Kaw
W.; Matsui, K.; Akakabe, Y.; Itai, N.; Kajiwara, T., Long-chain aldehyde-for
activity in tobacco leaves, Phytochemistry, 49(6), 1998, 1565-1568.)NIST
Spectranist ri

2166 (Program type: Complex; Column... (show more)class: Semi-standa
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Description: 40 0C (2 min) ^ 5 0C/min -> 80 0C ^ 7 oC/min -> 160 0C ^

0C/min -> 200 0C ^ 20 0C/min -> 280 0C (10 min); CAS no: 544354; Act

phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Au

Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparatio

identification of volatile compounds in Changyu XO brandy, Chinese J.

Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri

2171 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C

CAS no: 544354; Active phase: HP-5; Phase thickness: 0. 25 um; Data typ

Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao

EXtraction, preparation and identification of volatile compounds in Chang

brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist r

2152 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C

Heat rate: 5 K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start ti

min; CAS no: 544354; Active phase: HP-5; Carrier gas: He; Phase thickne

um; Data type: Normal alkane RI; Authors: Loizzo, M. R.; Tundis, R.; Conf

Saab, A. M.; Statti, G. A.; Menichini, F., Comparative chemical compositio

antioxidant and hypoglycaemic activities of Juniperus oxycedrus ssp. oxy

L. berry and wood oils from Lebanon, Food Chem., 105, 2007, 572-578.)N

Spectranist ri

2165 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: C

Heat rate: 4 K/min; Start T: 40 C; End T: 280 C; End time: 10 min; Start ti

min; CAS no: 544354; Active phase: Elite-5MS; Carrier gas: He; Phase thi

0. 5 um; Data type: Normal alkane RI; Authors: Tava, A.; Pecetti, L.; Ricci Pagnotta, M. A.; Russi, L., Volatile compounds from leaves and flowers of Bituminaria bituminosa (L.) Stirt. (Fabaceae) from Italy, Flavour Fragr. J., 2007, 363-370.)NIST Spectranist ri

2164 (Program type: Ramp; Column cl… (show more)ass: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start ti min; CAS no: 544354; Active phase: DB-5; Carrier gas: He; Phase thickne um; Data type: Normal alkane RI; Authors: Shen X.; Gao Y.; Su Q. D., Cor of the essential oil of Rhizoma polygonati, Flavour Fragr. J., 21, 2006, 556 558.)NIST Spectranist ri

2144 (Program type: Ramp; Column cl… (show more)ass: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 3 K/min; Start T: 60 C; End T: 280 C; CAS no: 544354; Active p HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal a Authors: Tzakou, O.; Said, A.; Farag, A.; Rashed, K., Volatile constituents Ailanthus excelsa Roxb., Flavour Fragr. J., 21, 2006, 899-901.)NIST Spect

2177 (Program type: Ramp; Column cl… (show more)ass: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 4. 3 K/min; Start T: 60 C; End T: 285 C; CAS no: 544354; Activ HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal a Authors: Tesevic, V.; Nikicevic, N.; Jovanovic, A.; Djokovic, D.; Vujisic, L.; Vuckovic, I.; Bonic, M., Volatile components from old plum brandies, Food

Technol. Biotechnol., 43(4), 2005, 367-372.)NIST Spectranist ri

2156 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: C
Heat rate: 4 K/min; Start T: 40 C; End T: 300 C; End time: 5 min; CAS no:
Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0. 25 um; Data
Normal alkane RI; Authors: Utsunomia, H.; Kawata, J.; Chanoki, W.; Shiral
Miyazawa, M., Components of Essential Oil from Woods of Prunus mume
Zucc., J. Oleo Sci., 54(11), 2005, 609-612.)NIST Spectranist ri

2161. 8 (Program type: Complex; Column... (show more)class: Semi-stan
non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty
Capillary; Description: 35C=> 5C/min => 220C=> 10C/min => 240C (5r
CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness
um; Data type: Normal alkane RI; Authors: Demyttenaere, J. C. R.; Sanch
Martinez, J. I.; Tellez Valdes, M. J.; Verhe, R.; Sandra, P., Analysis of volati
of malt whisky using solid phase microextraction and dynamic headspac
25th International Symposium on Capillary Chromatography, 2002, 1-13.
Spectranist ri

2155 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 3 K/min; Start T: 60 C; End T: 270 C; CAS no: 544354; Active p
DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alka
Authors: Palmeira, S. F., Jr.; Conserva, L. M.; Andrade, E. H. A.; Guilhon, G
P., Analysis by GC-MS of the hexane extract of the aerial parts of Aristolo

acutifolia Duchtr., Flavour Fragr. J., 16, 2001, 85-88.)NIST Spectranist ri

2515 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
no: 544354; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness
um; Data type: Normal alkane RI; Authors: Zhao, Y.; Xu, Y.; Li, J.; Fan, W.
W., Profile of volatile compounds in 11 brandies by headspace solid-phas
microextraction followed by gas chromatography-mass spectrometry, J. F
Sci., 74(2), 2009, c90-c99.)NIST Spectranist ri

2532 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 3 K/min; Start T: 40 C; End T: 230 C; End time: 5 min; Start time: 2
no: 544354; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness
um; Data type: Normal alkane RI; Authors: Zhao, Y.; Xu, Y.; Li, J.; Fan, W.
W., Profile of volatile compounds in 11 brandies by headspace solid-phas
microextraction followed by gas chromatography-mass spectrometry, J. F
Sci., 74(2), 2009, c90-c99.)NIST Spectranist ri

2511 (Program type: Complex; Column... (show more)class: Standard po
Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capilla
Description: 60 0C (3 min) ^ 2 0C/min -> 220 0C ^ 3 0C/min -> 245 0C (
CAS no: 544354; Active phase: DB-Wax; Carrier gas: Hydrogen; Phase th
0. 50 um; Data type: Normal alkane RI; Authors: Selli, S., Volatile constitu
orange obtained from moro oranges (Citrus Sinensis L. Osbeck), J. Food C
30, 2007, 330-341.)NIST Spectranist ri

2530 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column type: Capillary; CAS no: 544354; Active phase: Carbowax 20M; D
type: Normal alkane RI; Authors: Vinogradov, B. A., Production, composit
properties and application of essential oils, 2004.)NIST Spectranist ri

2538 (Program type: Complex; Column... (show more)class: Standard po
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
Description: 60C(10min) => 4C/min => 220C(10min) => 1C/min => 24
no: 544354; Active phase: HP-Innowax FSC; Carrier gas: He; Phase thickn
25 um; Data type: Normal alkane RI; Authors: Erdemoglu, N.; Sener, B.; D
B.; Baser, K. H. C., The glycosidically bound volatile compounds of Taxus
Chem. Nat. Compd. (Engl. Transl.), 39(2), 2003, 195-198, In original 147-
149.)NIST Spectranist ri

2528 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
rate: 4 K/min; Start T: 80 C; End T: 250 C; End time: 30 min; CAS no: 544
Active phase: TC-Wax; Carrier gas: He; Data type: Normal alkane RI; Autl
Miyazawa, M.; Okuno, Y., Volatile components from the roots of Scrophul
ningpoensis Hemsl., Flavour Fragr. J., 18, 2003, 398-400.)NIST Spectranis

2486 (Program type: Complex; Column... (show more)class: Standard po
Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capilla
Description: 45C(5min)=> 20C/min => 100C(1min)=> 3C/min => 190C
CAS no: 544354; Active phase: Nukol; Carrier gas: N2; Data type: Norma
RI; Authors: Lopez, M. G.; Dufour, J. P., Chapter 6. Tequilas: charm analys
Blanco, Teposado, and Anejo tequilas, Am. Chem. Soc. Symp. Ser., 782, 2

62-72.)NIST Spectranist ri

2520 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
rate: 4 K/min; Start T: 80 C; End T: 250 C; End time: 47 min; CAS no: 544
Active phase: TC-Wax; Carrier gas: He; Data type: Normal alkane RI; Autl
Miyazawa, M.; Kurose, K.; Itoh, A.; Hiraoka, N., Comparison of the essenti
Glehnia littoralis from Northern and Southern Japan, J. Agric. Food Chem.
2001, 5433-5436.)NIST Spectranist ri

2521 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
rate: 2 K/min; Start T: 40 C; End T: 200 C; Start time: 2 min; CAS no: 544
Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data
Normal alkane RI; Authors: Umano, K.; Hagi, Y.; Nakahara, K.; Shoji, A.;
Shibamoto, T., Volatile chemicals identified in extracts from leaves of Jap
mugwort (Artemisia princeps Pamp.), J. Agric. Food Chem., 48, 2000, 346
3469.)NIST Spectranist ri

2505 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capilla
rate: 2 K/min; Start T: 60 C; End T: 190 C; End time: 21 min; Start time: 4
CAS no: 544354; Active phase: CP-Wax 52CB; Carrier gas: H2; Phase thic
0. 22 um; Data type: Normal alkane RI; Authors: Hwan, C.-H.; Chou, C.-C.
components of the Chinese fermented soya bean curd as affected by the
of ethanol in ageing solution, J. Sci. Food Agric., 79, 1999, 243-248.)NIST

Spectranist ri

2536 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
T: 60 C; End T: 220 C; Start time: 10 min; CAS no: 544354; Active phase:
Innowax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal
RI; Authors: Kaya, A.; Baser, K. H. C.; Demirci, B.; Koca, F., The essential
Acinos alpinus (L.) Moench growing in Turkey, Flavour Fragr. J., 14, 1999,
59.)NIST Spectranist ri

2534 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
rate: 3 K/min; Start T: 80 C; End T: 240 C; Start time: 5 min; CAS no: 544
Active phase: TC-Wax; Data type: Normal alkane RI; Authors: Shuichi, H.;
Masazumi, N.; Hiromu, K.; Kiyoshi, F., Comparison of volatile compounds
the crude drugs, Onji-tsutsu and Onji-niki, Nippon nogei kagaku kaishi, 7
1996, 151-160.)NIST Spectranist ri

- **Retention Index (Linear):**

2139 (Program type: Ramp; Column cl... (show more)ass: Standard non-p
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 5 K/min; Start T: 50 C; End T: 250 C; End time: 15 min; Start time: 3
CAS no: 544354; Active phase: SPB-1; Carrier gas: He; Phase thickness: 0
Data type: Linear RI; Authors: Blagojevic, P.; Radulovic, N.; Palic, R.; Stoja
G., Chemical composition of the essential oils of Serbian wild-growing Srt
absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-
Program type: Ramp; Column cl... (show more)ass: Standard non-polar; C

diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 280 C; End time: 10 min; CAS no: 544354; Ac
phase: OV-1; Carrier gas: He; Data type: Linear RI; Authors: Tan, S.-T.; H
T.; Wilkins, A. L.; Molan, P. C., Extractives from New Zealand honeys. 1. V
clovers, manuka, and kanuka unifloral honeys, J. Agric. Food Chem., 36,
453-460.)NIST Spectranist ri

2177 (Program type: Ramp; Column cl... (show more)ass: Standard non-
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 16 K/min; Start T: 60 C; End T: 280 C; End time: 10 min; Start time:
CAS no: 544354; Active phase: SE-30; Carrier gas: He; Phase thickness:
Data type: Linear RI; Authors: Tundis, R.; Passalacqua, N. G.; Peruzzi, L.;
A.; Bonesi, M.; Loizzo, M. R.; Conforti, F.; Cesca, G.; Menichini, F., Compa
chemical variability of the non-polar extracts from Senecio cineraria grou
(Asteraceae), Biochem. Syst. Ecol., 33, 2005, 1071-1076.)NIST Spectrani

2162 (Program type: Ramp; Column cl... (show more)ass: Standard non-
Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla
rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 1
CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickn
25 um; Data type: Linear RI; Authors: Pino, J.; Almora, K.; Marbot, R., Vola
components of papaya (Carica papaya L., maradol variety) fruit, Flavour
18, 2003, 492-496.)NIST Spectranist ri

2145 (Program type: Ramp; Column cl... (show more)ass: Standard non-
Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capilla
rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 1

CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickn

um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C.,

Characterization of volatile in Cosa Rican Guava [Psidium friedrichsthalia

(Berg) Niedenzu] fruit, J. Agric. Food Chem., 50, 2002, 6023-6026.)NIST

Spectranist ri

2141 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capilla

rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 1

CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickn

um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R., Volatile flavor

constituents of acerola (Malpighia emarginata DC.) fruit, J. Agric. Food Ch

2001, 5880-5882., Program type: Ramp; Column cl... (show more)ass: St

non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column ty

Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 m

time: 10 min; CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He

thickness: 0. 4 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; V

C., Characterization of volatiles in strawberry guava (Psidium cattleianum

Sabine) fruit, J. Agric. Food Chem., 49, 2001, 5883-5887.)NIST Spectranis

2155 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0. 2 mm; Column length: 30 m; Column type: Ca

Heat rate: 5 K/min; Start T: 50 C; End T: 250 C; End time: 15 min; Start ti

min; CAS no: 544354; Active phase: DB-5; Carrier gas: He; Phase thickne

um; Data type: Linear RI; Authors: Blagojevic, P.; Radulovic, N.; Palic, R.;

Stojanovic, G., Chemical composition of the essential oils of Serbian wild-

Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 20
4780-4789.)NIST Spectranist ri

2159 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 4 K/min; Start T: 60 C; End T: 250 C; End time: 20 min; Start ti
min; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thick
25 um; Data type: Linear RI; Authors: Pino, J. A.; Mesa, J.; Munoz, Y.; Mart
Marbot, R., Volatile components from mango (Mangifera indica L.) cultiva
Agric. Food Chem., 53, 2005, 2213-2223., Program type: Ramp; Column
(show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm;
length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 60 C; E
250 C; End time: 20 min; Start time: 2 min; CAS no: 544354; Active phas
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors
A.; Marbot, R.; Vazquez, C., Volatile components of tamarind (Tamarindu
L.) grown in Cuba, J. Essent. Oil Res., 16, 2004, 318-320.)NIST Spectranis

2151 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 5 K/min; Start T: 50 C; End T: 250 C; End time: 5 min; Start tim
min; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thick
25 um; Data type: Linear RI; Authors: Shang, C.; Hu, Y.; Deng, C.; Hu, K.,
determination of volatile constituents of Michelia alba flowers by gas
chromatography-mass spectrometry with solid-phase microextraction, J.
Chromatogr. A, 942, 2002, 283-288.)NIST Spectranist ri

2519 (Program type: Ramp; Column cl... (show more)ass: Standard polar

Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla

rate: 6 K/min; Start T: 35 C; End T: 195 C; End time: 60 min; Start time: 5

CAS no: 544354; Active phase: Supelcowax-10; Phase thickness: 0. 25 u

type: Linear RI; Authors: Chung, H. Y.; Fung, P. K.; Kim, J.-S., Aroma impa

components in commercial plain sufu, J. Agric. Food Chem., 53, 2005, 16

1691.)NIST Spectranist ri

2524 (Program type: Ramp; Column cl… (show more)ass: Standard polar

Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla

rate: 1. 8 K/min; Start T: 35 C; End T: 220 C; End time: 10 min; Start time

min; CAS no: 544354; Active phase: ZB-Wax; Carrier gas: He; Phase thick

15 um; Data type: Linear RI; Authors: Ledauphin, J.; Saint-Clair, J.-F.; Labl

O.; Guichard, H.; Founier, N.; Guichard, E.; Barillier, D., Identification of tr

volatile compounds in freshly distilled calvados and cognac using prepara

separations coupled with gas chromatography-mass spectrometry, J. Agr

Chem., 52, 2004, 5124-5134.)NIST Spectranist ri

2553 (Program type: Ramp; Column cl… (show more)ass: Standard polar

Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capilla

rate: 4 K/min; Start T: 35 C; End T: 225 C; End time: 10 min; Start time: 5

CAS no: 544354; Active phase: Supelcowax; Phase thickness: 0. 25 um; D

type: Linear RI; Authors: Chisholm, M. G.; Wilson, M. A.; Gaskey, G. M.,

Characterization of aroma volatiles in key lime essential oils (Cirtrus aura

Swingle), Flavour Fragr. J., 18, 2003, 106-115.)NIST Spectranist ri

2514 (Program type: Ramp; Column cl… (show more)ass: Standard polar

Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla

rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 1

CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness

um; Data type: Linear RI; Authors: Pino, J.; Almora, K.; Marbot, R., Volatile

components of papaya (Carica papaya L., maradol variety) fruit, Flavour

18, 2003, 492-496.)NIST Spectranist ri

2491 (Program type: Ramp; Column cl... (show more)ass: Standard polar

Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla

rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 1

CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness

um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C.,

Characterization of volatile in Cosa Rican Guava [Psidium friedrichsthalia

(Berg) Niedenzu] fruit, J. Agric. Food Chem., 50, 2002, 6023-6026., Progr

Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0

Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T

End T: 250 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Act

phase: AT-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Li

Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Characterization of volatiles

strawberry guava (Psidium cattleianum Sabine) fruit, J. Agric. Food Chem

2001, 5883-5887.)NIST Spectranist ri

2510 (Program type: Complex; Column... (show more)class: Standard po

Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla

Description: 20C(30s) => fast=> 60C => 4C/min => 220C (20min); CAS

544354; Active phase: DB-Wax; Phase thickness: 0. 25 um; Data type: Li

Authors: Cantergiani, E.; Brevard, H.; Krebs, Y.; Feria-Morales, A.; Amado

Yeretzian, C., Characterisation of the aroma of green Mexican coffee and identification of mouldy/earthy defect, Eur. Food Res. Technol., 212, 200 657.)NIST Spectranist ri

2488 (Program type: Ramp; Column cl... (show more)ass: Standard polar Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 1 CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R., Volatile flavor constituents of acerola (Malpighia emarginata DC.) fruit, J. Agric. Food Ch 2001, 5880-5882.)NIST Spectranist ri

2530 (Program type: Ramp; Column cl... (show more)ass: Standard polar Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; CAS no: 544 Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um type: Linear RI; Authors: Chung, H. Y., Volatile flavor components in red fermented soybean (Glycine max) curds, J. Agric. Food Chem., 48, 2000, 1809., Program type: Ramp; Column cl... (show more)ass: Standard pola Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; Start time: 5 CAS no: 544354; Active phase: Supelcowax-10; Carrier gas: He; Phase th 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y., Volatile componen fermented soybean (Glycine max) curds, J. Agric. Food Chem., 47, 1999, 2696.)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:	388. 3±21. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 9 mmHg at 25°C
Enthalpy of Vaporization:	63. 7±3. 0 kJ/mol
Flash Point:	96. 3±20. 4 °C
Index of Refraction:	1. 465
Molar Refractivity:	96. 6±0. 3 cm ^{3}
#H bond acceptors:	2
#H bond donors:	0
#Freely Rotating Bonds:	16
#Rule of 5 Violations:	1
ACD/LogP:	8. 17
ACD/LogD (pH 5. 5):	7. 46
ACD/BCF (pH 5. 5):	274087. 41
ACD/KOC (pH 5. 5):	271653. 47

ACD/LogD (pH 7. 4):	7. 46
ACD/BCF (pH 7. 4):	274087. 41
ACD/KOC (pH 7. 4):	271653. 47
Polar Surface Area:	26 Å ^{2}
Polarizability:	38. 3±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	31. 4±3. 0 dyne/cm
Molar Volume:	349. 4±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) = 8. 29Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 367. 74 (Adapted Stein & Brown method)Melting Pt (deg C): 87. 62 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 99E-005 (Modified Grain method)MP (exp database): 8 at 25 deg C : 2. 848E-002 L/mol-secKb Half-Life at pH 8: 281. 632 days Kb Half-Life at pH 7: 7. 711 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 540 (BCF = 34. 69)log Kow used: 8. 29 (estimated)Volatilization from Water: Henry LC: 0. 00274 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 2. 168 hoursHalf-Life from Model Lake : 170. 9 hours (7. 122 days)Removal In Wastewater Treatment: Total removal: 94. 03 percentTotal biodegradation: 0. 78 percentTotal sludge adsorption: 93. 24 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0267 0. 69 1000 Water 3. 77 360 1000 Soil 28. 1 720 1000 Sediment 68. 1 3. 24e+003 0 Persistence Time: 1. 23e+003 hr

Click to predict properties on the Chemicalize site