

# [Ethyl linoleate (jan) c20h36o2 structure](https://assignbuster.com/ethyl-linoleate-jan-c20h36o2-structure/)

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* Retention Index (Linear):

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| --- | --- |
| 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):

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| 2193 (estimated with error: 47)NIST Spectramainlib\_155747, replib\_229299, replib\_55769  |

## Retention Index (Normal Alkane):

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| 2159 (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: 40 C; End T: 250 C; End time: 10 min; Start time: 5 min; CAS no: 544354; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Loizzo, M. R.; Tundis, R.; Conforti, F.; Saab, A. M.; Statti, G. A.; Menichini, F., Comparative chemical composition, antioxidant and hypoglycaemic activities of Juniperus oxycedrus ssp. oxycedrus L. berry and wood oils from Lebanon, Food Chem., 105, 2007, 572-578.)NIST Spectranist ri  |
| 2140 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 544354; Active phase: SE-30; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production, composition, properties and application of essential oils, 2004.)NIST Spectranist ri  |
| 2162 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 35C=> 5C/min => 160C=> 10C/min => 220C (10min); CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Demyttenaere, J. C. R.; Sanchez Martinez, J. I.; Tellez Valdes, M. J.; Verhe, R.; Sandra, P., Analysis of volatile esters of malt whisky using solid phase microextraction and dynamic headspace, in 25th International Symposium on Capillary Chromatography, 2002, 1-13., Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 35C=> 5C/min=> 220C=> 10C/min=> 240C(5min); CAS no: 544354; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Demyttenaere, J. C. R.; Sanchez Martinez, J. I.; Verhe, R.; Sandra, P.; de Kimpe, N., Analysis of volatiles of malt whisky by solid-phase microextraction and stir bar sorptive extraction, J. Chromatogr. A, 985, 2003, 221-232., Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 28 mm; Column length: 40 m; Column type: Capillary; Description: 75C => 3C/min => 190C(25min) => 3C/min => 210C; CAS no: 544354; Active phase: SF-96; Data type: Normal alkane RI; Authors: Kawasaki, W.; Matsui, K.; Akakabe, Y.; Itai, N.; Kajiwara, T., Long-chain aldehyde-forming activity in tobacco leaves, Phytochemistry, 49(6), 1998, 1565-1568.)NIST Spectranist ri  |
| 2166 (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: 544354; 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  |
| 2171 (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: 544354; 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  |
| 2152 (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: 40 C; End T: 250 C; End time: 10 min; Start time: 5 min; CAS no: 544354; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Loizzo, M. R.; Tundis, R.; Conforti, F.; Saab, A. M.; Statti, G. A.; Menichini, F., Comparative chemical composition, antioxidant and hypoglycaemic activities of Juniperus oxycedrus ssp. oxycedrus L. berry and wood oils from Lebanon, Food Chem., 105, 2007, 572-578.)NIST Spectranist ri  |
| 2165 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 280 C; End time: 10 min; Start time: 5 min; CAS no: 544354; Active phase: Elite-5MS; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Tava, A.; Pecetti, L.; Ricci, M.; Pagnotta, M. A.; Russi, L., Volatile compounds from leaves and flowers of Bituminaria bituminosa (L.) Stirt. (Fabaceae) from Italy, Flavour Fragr. J., 22, 2007, 363-370.)NIST Spectranist ri  |
| 2164 (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: 4 K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start time: 2 min; CAS no: 544354; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shen X.; Gao Y.; Su Q. D., Constituents 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 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: 280 C; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Tzakou, O.; Said, A.; Farag, A.; Rashed, K., Volatile constituents of Ailanthus excelsa Roxb., Flavour Fragr. J., 21, 2006, 899-901.)NIST Spectranist ri  |
| 2177 (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: 4. 3 K/min; Start T: 60 C; End T: 285 C; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; 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 non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 300 C; End time: 5 min; CAS no: 544354; Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Utsunomia, H.; Kawata, J.; Chanoki, W.; Shirakawa, N.; Miyazawa, M., Components of Essential Oil from Woods of Prunus mume Sieb. at Zucc., J. Oleo Sci., 54(11), 2005, 609-612.)NIST Spectranist ri  |
| 2161. 8 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 35C=> 5C/min => 220C=> 10C/min => 240C (5min); CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Demyttenaere, J. C. R.; Sanchez Martinez, J. I.; Tellez Valdes, M. J.; Verhe, R.; Sandra, P., Analysis of volatile esters of malt whisky using solid phase microextraction and dynamic headspace, in 25th International Symposium on Capillary Chromatography, 2002, 1-13.)NIST Spectranist ri  |
| 2155 (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: 270 C; CAS no: 544354; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Palmeira, S. F., Jr.; Conserva, L. M.; Andrade, E. H. A.; Guilhon, G. M. S. P., Analysis by GC-MS of the hexane extract of the aerial parts of Aristolochia 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: Capillary; CAS no: 544354; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Xu, Y.; Li, J.; Fan, W.; Jiang, W., Profile of volatile compounds in 11 brandies by headspace solid-phase microextraction followed by gas chromatography-mass spectrometry, J. Food. 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: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 230 C; End time: 5 min; Start time: 2 min; CAS no: 544354; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Xu, Y.; Li, J.; Fan, W.; Jiang, W., Profile of volatile compounds in 11 brandies by headspace solid-phase microextraction followed by gas chromatography-mass spectrometry, J. Food. Sci., 74(2), 2009, c90-c99.)NIST Spectranist ri  |
| 2511 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 60 0C (3 min) ^ 2 0C/min -> 220 0C ^ 3 0C/min -> 245 0C (20 min); CAS no: 544354; Active phase: DB-Wax; Carrier gas: Hydrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Selli, S., Volatile constituents of orange obtained from moro oranges (Citrus Sinensis L. Osbeck), J. Food Quality, 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; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production, composition, properties and application of essential oils, 2004.)NIST Spectranist ri  |
| 2538 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Description: 60C(10min) => 4C/min => 220C(10min) => 1C/min => 240C; CAS no: 544354; Active phase: HP-Innowax FSC; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Erdemoglu, N.; Sener, B.; Demirci, B.; Baser, K. H. C., The glycosidically bound volatile compounds of Taxus baccata, 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: Capillary; Heat rate: 4 K/min; Start T: 80 C; End T: 250 C; End time: 30 min; CAS no: 544354; Active phase: TC-Wax; Carrier gas: He; Data type: Normal alkane RI; Authors: Miyazawa, M.; Okuno, Y., Volatile components from the roots of Scrophularia ningpoensis Hemsl., Flavour Fragr. J., 18, 2003, 398-400.)NIST Spectranist ri  |
| 2486 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capillary; Description: 45C(5min)=> 20C/min => 100C(1min)=> 3C/min => 190C(40min); CAS no: 544354; Active phase: Nukol; Carrier gas: N2; Data type: Normal alkane RI; Authors: Lopez, M. G.; Dufour, J. P., Chapter 6. Tequilas: charm analysis of Blanco, Teposado, and Anejo tequilas, Am. Chem. Soc. Symp. Ser., 782, 2001, 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: Capillary; Heat rate: 4 K/min; Start T: 80 C; End T: 250 C; End time: 47 min; CAS no: 544354; Active phase: TC-Wax; Carrier gas: He; Data type: Normal alkane RI; Authors: Miyazawa, M.; Kurose, K.; Itoh, A.; Hiraoka, N., Comparison of the essential oils of Glehnia littoralis from Northern and Southern Japan, J. Agric. Food Chem., 49, 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: Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 200 C; Start time: 2 min; CAS no: 544354; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Umano, K.; Hagi, Y.; Nakahara, K.; Shoji, A.; Shibamoto, T., Volatile chemicals identified in extracts from leaves of Japanese mugwort (Artemisia princeps Pamp.), J. Agric. Food Chem., 48, 2000, 3463-3469.)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: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 190 C; End time: 21 min; Start time: 4 min; CAS no: 544354; Active phase: CP-Wax 52CB; Carrier gas: H2; Phase thickness: 0. 22 um; Data type: Normal alkane RI; Authors: Hwan, C.-H.; Chou, C.-C., Volatile components of the Chinese fermented soya bean curd as affected by the addition 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: Capillary; Start 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 alkane RI; Authors: Kaya, A.; Baser, K. H. C.; Demirci, B.; Koca, F., The essential oil of Acinos alpinus (L.) Moench growing in Turkey, Flavour Fragr. J., 14, 1999, 55-59.)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: Capillary; Heat rate: 3 K/min; Start T: 80 C; End T: 240 C; Start time: 5 min; CAS no: 544354; Active phase: TC-Wax; Data type: Normal alkane RI; Authors: Shuichi, H.; Masazumi, N.; Hiromu, K.; Kiyoshi, F., Comparison of volatile compounds berween the crude drugs, Onji-tsutsu and Onji-niki, Nippon nogei kagaku kaishi, 70(2), 1996, 151-160.)NIST Spectranist ri  |

## Retention Index (Linear):

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| 2139 (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: 250 C; End time: 15 min; Start time: 3 min; CAS no: 544354; Active phase: SPB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 40 C; End T: 280 C; End time: 10 min; CAS no: 544354; Active phase: OV-1; Carrier gas: He; Data type: Linear RI; Authors: Tan, S.-T.; Holland, P. T.; Wilkins, A. L.; Molan, P. C., Extractives from New Zealand honeys. 1. White clovers, manuka, and kanuka unifloral honeys, J. Agric. Food Chem., 36, 1988, 453-460.)NIST Spectranist ri  |
| 2177 (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: 16 K/min; Start T: 60 C; End T: 280 C; End time: 10 min; Start time: 3 min; CAS no: 544354; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Tundis, R.; Passalacqua, N. G.; Peruzzi, L.; Statti, G. A.; Bonesi, M.; Loizzo, M. R.; Conforti, F.; Cesca, G.; Menichini, F., Comparative chemical variability of the non-polar extracts from Senecio cineraria group (Asteraceae), Biochem. Syst. Ecol., 33, 2005, 1071-1076.)NIST Spectranist ri  |
| 2162 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J.; Almora, K.; Marbot, R., Volatile components of papaya (Carica papaya L., maradol variety) fruit, Flavour Fragr. J., 18, 2003, 492-496.)NIST Spectranist ri  |
| 2145 (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: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Characterization of volatile in Cosa Rican Guava [Psidium friedrichsthalianum (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-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R., Volatile flavor constituents of acerola (Malpighia emarginata DC.) fruit, J. Agric. Food Chem., 49, 2001, 5880-5882., 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: 3 K/min; Start T: 60 C; End T: 280 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Characterization of volatiles in strawberry guava (Psidium cattleianum Sabine) fruit, J. Agric. Food Chem., 49, 2001, 5883-5887.)NIST Spectranist ri  |
| 2155 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 250 C; End time: 15 min; Start time: 3 min; CAS no: 544354; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789.)NIST Spectranist ri  |
| 2159 (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: 4 K/min; Start T: 60 C; End T: 250 C; End time: 20 min; Start time: 2 min; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Mesa, J.; Munoz, Y.; Marti, M. P.; Marbot, R., Volatile components from mango (Mangifera indica L.) cultivars, J. Agric. Food Chem., 53, 2005, 2213-2223., 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: 4 K/min; Start T: 60 C; End T: 250 C; End time: 20 min; Start time: 2 min; CAS no: 544354; Active phase: SPB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Volatile components of tamarind (Tamarindus indica L.) grown in Cuba, J. Essent. Oil Res., 16, 2004, 318-320.)NIST Spectranist ri  |
| 2151 (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: 50 C; End T: 250 C; End time: 5 min; Start time: 2 min; CAS no: 544354; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Shang, C.; Hu, Y.; Deng, C.; Hu, K., Rapid 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: Capillary; Heat rate: 6 K/min; Start T: 35 C; End T: 195 C; End time: 60 min; Start time: 5 min; CAS no: 544354; Active phase: Supelcowax-10; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y.; Fung, P. K.; Kim, J.-S., Aroma impact components in commercial plain sufu, J. Agric. Food Chem., 53, 2005, 1684-1691.)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: Capillary; Heat rate: 1. 8 K/min; Start T: 35 C; End T: 220 C; End time: 10 min; Start time: 10 min; CAS no: 544354; Active phase: ZB-Wax; Carrier gas: He; Phase thickness: 0. 15 um; Data type: Linear RI; Authors: Ledauphin, J.; Saint-Clair, J.-F.; Lablanquie, O.; Guichard, H.; Founier, N.; Guichard, E.; Barillier, D., Identification of trace volatile compounds in freshly distilled calvados and cognac using preparative separations coupled with gas chromatography-mass spectrometry, J. Agric. Food 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: Capillary; Heat rate: 4 K/min; Start T: 35 C; End T: 225 C; End time: 10 min; Start time: 5 min; CAS no: 544354; Active phase: Supelcowax; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chisholm, M. G.; Wilson, M. A.; Gaskey, G. M., Characterization of aroma volatiles in key lime essential oils (Cirtrus aurantifolia 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: Capillary; Heat rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J.; Almora, K.; Marbot, R., Volatile components of papaya (Carica papaya L., maradol variety) fruit, Flavour Fragr. J., 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: Capillary; Heat rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Characterization of volatile in Cosa Rican Guava [Psidium friedrichsthalianum (Berg) Niedenzu] fruit, J. Agric. Food Chem., 50, 2002, 6023-6026., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Vazquez, C., Characterization of volatiles in strawberry guava (Psidium cattleianum Sabine) fruit, J. Agric. Food Chem., 49, 2001, 5883-5887.)NIST Spectranist ri  |
| 2510 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 20C(30s) => fast=> 60C => 4C/min => 220C (20min); CAS no: 544354; Active phase: DB-Wax; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Cantergiani, E.; Brevard, H.; Krebs, Y.; Feria-Morales, A.; Amado, R.; Yeretzian, C., Characterisation of the aroma of green Mexican coffee and identification of mouldy/earthy defect, Eur. Food Res. Technol., 212, 2001, 648-657.)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: Capillary; Heat rate: 2 K/min; Start T: 65 C; End T: 250 C; End time: 60 min; Start time: 10 min; CAS no: 544354; Active phase: AT-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R., Volatile flavor constituents of acerola (Malpighia emarginata DC.) fruit, J. Agric. Food Chem., 49, 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: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; CAS no: 544354; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y., Volatile flavor components in red fermented soybean (Glycine max) curds, J. Agric. Food Chem., 48, 2000, 1803-1809., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 195 C; End time: 90 min; Start time: 5 min; CAS no: 544354; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y., Volatile components in fermented soybean (Glycine max) curds, J. Agric. Food Chem., 47, 1999, 2690-2696.)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

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