

# [2,4-octadienal c8h12o structure](https://assignbuster.com/24-octadienal-c8h12o-structure/)

Contents

* Retention Index (Linear):

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| --- | --- |
| Molecular Formula  | C 8 H 12 O  |
| Average mass  | 124. 180 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 198. 2±9. 0 °C at 760 mmHg  |
| Flash Point  | 83. 0±11. 0 °C  |
| Molar Refractivity  | 39. 4±0. 3 cm 3  |
| Polarizability  | 15. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 28. 0±3. 0 dyne/cm  |
| Molar Volume  | 145. 1±3. 0 cm 3  |

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

## Experimental Boiling Point:

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| --- |
| 105-106 °C / 8 mm Hg (266. 0737-267. 4609 °C / 760 mmHg)Food and Agriculture Organization of the United Nations(2E, 4E)-Octa-2, 4-dienal  |
| 11 °C / 83 mmHg (72. 4079 °C / 760 mmHg)FooDBFDB008349  |

## Experimental Refraction Index:

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| --- |
| 1. 519-1. 525Food and Agriculture Organization of the United Nations(2E, 4E)-Octa-2, 4-dienal  |
| 20FooDBFDB008349  |

* Miscellaneous

## Appearance:

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| Liquid; fatty, green, sour aromaFood and Agriculture Organization of the United Nations(2E, 4E)-Octa-2, 4-dienal  |

* Gas Chromatography

## Retention Index (Kovats):

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| 1021 (estimated with error: 45)NIST Spectramainlib\_249490, replib\_57735  |

## Retention Index (Normal Alkane):

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| --- |
| 1086 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary; Description: 35C(3min) => 4C/min=> 190C => 30C/min => 225C(3min); CAS no: 30361285; Active phase: HP-1; Phase thickness: 0. 11 um; Data type: Normal alkane RI; Authors: Carpino, S.; Mallia, S.; La Terra, S.; Melilli, C.; Licitra, G.; Acree, T. E.; Barbano, D. M.; van Soest, P. J., Composition and aroma compounds of ragusano cheese: native pasture and total mixed rations, J. Dairy Sci., 87(4), 2004, 816-830., Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 12 m; Column type: Capillary; Description: 35C(3min)=> 6C/min=> 190C=> 30C/min => 225C; CAS no: 30361285; Active phase: HP-1; Phase thickness: 0. 52 um; Data type: Normal alkane RI; Authors: Carpino, S.; Mallia, S.; Licitra, G.; van Soest, P. J.; Acree, T. E., Aroma compounds of some Hyblean pasture species, Flavour Fragr. J., 19, 2004, 293-297.)NIST Spectranist ri  |
| 1087 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 30361285; Active phase: OV-101; Carrier gas: N2; Data type: Normal alkane RI; Authors: Tamura, H.; Nakamoto, H.; Yang, R.-H.; Sugisawa, H., Characteristic aroma compounds in green algae (Ulva pertusa) volatiles, Nippon Shokuhin Kagaku Kogaku Kaishi, 42(11), 1995, 887-891.)NIST Spectranist ri  |
| 1090 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 30361285; Active phase: OV-101; Carrier gas: N2; Data type: Normal alkane RI; Authors: Tamura, H.; Nakamoto, H.; Yang, R.-H.; Sugisawa, H., Characteristic aroma compounds in green algae (Ulva pertusa) volatiles, Nippon Shokuhin Kagaku Kogaku Kaishi, 42(11), 1995, 887-891.)NIST Spectranist ri  |
| 1088 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 70 C; End T: 200 C; CAS no: 30361285; Active phase: OV-101; Carrier gas: Nitrogen; Data type: Normal alkane RI; Authors: Sugisawa, H.; Nakamura, K.; Tamura, H., The aroma profile of the volatile in marine green algae (Ulva pertusa), Food Reviews International, 6(4), 1990, 573-589., Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 30361285; Active phase: OV-101; Carrier gas: Nitrogen; Data type: Normal alkane RI; Authors: Sugisawa, H.; Nakamura, K.; Tamura, H., The aroma profile of the volatile in marine green algae (Ulva pertusa), Food Reviews International, 6(4), 1990, 573-589.)NIST Spectranist ri  |
| 1108 (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: 6 K/min; Start T: 40 C; End T: 230 C; End time: 20 min; Start time: 2 min; CAS no: 30361285; Active phase: DB-5 MS; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Chen, G.; Song, H.; Ma, C., Aroma-active aompounds of Beijing roast duck, Flavour Fragr. J., 24, 2009, 186-191.)NIST Spectranist ri  |
| 1110 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(2min) => 40C/min => 60C(2min) => 6C/min => 180C => 15C/min => 230C(10min); CAS no: 30361285; Active phase: DB-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Buettner, A., A selective and sensitive approach to characterize odour-active and volatile constituents in small-scale human milk samples, Flavour Fragr. J., 22, 2007, 465-473.)NIST Spectranist ri  |
| 1605 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 60 C; End T: 200 C; End time: 9. 5 min; Start time: 3 min; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintreau, A., Strategy for the identification of key odorants: application to shrimp aroma, J. Chromatogr. A, 1216, 2009, 6424-6432.)NIST Spectranist ri  |
| 1628 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 60 C; End T: 200 C; End time: 9. 5 min; Start time: 3 min; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintreau, A., Strategy for the identification of key odorants: application to shrimp aroma, J. Chromatogr. A, 1216, 2009, 6424-6432.)NIST Spectranist ri  |
| 1632 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 60 C; End T: 200 C; End time: 9. 5 min; Start time: 3 min; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintreau, A., Strategy for the identification of key odorants: application to shrimp aroma, J. Chromatogr. A, 1216, 2009, 6424-6432., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 240 C; End time: 20 min; Start time: 2 min; CAS no: 30361285; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 1 um; Data type: Normal alkane RI; Authors: Rochat, S.; Chaintreau, A., Carbonyl Odorants Contributing to the In-Oven Roast Beef Top Note, J. Agric. Food Chem., 53, 2005, 9578-9585.)NIST Spectranist ri  |
| 1585 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(2min) => 40C/min => 60C(2min) => 6C/min => 180C => 15C/min => 230C(10min); CAS no: 30361285; Active phase: DB-FFAP; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Buettner, A., A selective and sensitive approach to characterize odour-active and volatile constituents in small-scale human milk samples, Flavour Fragr. J., 22, 2007, 465-473.)NIST Spectranist ri  |
| 1601 (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: 210 C; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Kumazawa, K.; Wada, Y.; Masuda, H., Characterization of epoxydecenal isomers as potent odorants in black tea (Dimbula) infusion, J. Agric. Food Chem., 54, 2006, 4795-4801.)NIST Spectranist ri  |
| 1630 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 240 C; End time: 20 min; Start time: 2 min; CAS no: 30361285; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 1 um; Data type: Normal alkane RI; Authors: Rochat, S.; Chaintreau, A., Carbonyl Odorants Contributing to the In-Oven Roast Beef Top Note, J. Agric. Food Chem., 53, 2005, 9578-9585.)NIST Spectranist ri  |
| 1634 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 240 C; End time: 20 min; Start time: 2 min; CAS no: 30361285; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 1 um; Data type: Normal alkane RI; Authors: Rochat, S.; Chaintreau, A., Carbonyl Odorants Contributing to the In-Oven Roast Beef Top Note, J. Agric. Food Chem., 53, 2005, 9578-9585.)NIST Spectranist ri  |
| 1595 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Description: 50C(6min) => 1C/min => 130C => 10C/min => 240C (15min); CAS no: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Piveteau, F.; le Guen, S.; Gandemer, G.; Baud, J.-P.; Demaimay, M., Aroma of fresh oysters Crassostrea gigas: composition and aroma notes, J. Agric. Food Chem., 48, 2000, 4851-4857.)NIST Spectranist ri  |
| 1557 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 180 C; Start time: 4 min; CAS no: 30361285; Active phase: Carbowax 20M; Carrier gas: He; Data type: Normal alkane RI; Authors: Kawakami, M.; Kobayashi, A., Volatitle constituents of greem mate and roasted mate, J. Agric. Food Chem., 39(7), 1991, 1275-1279.)NIST Spectranist ri  |
| 1590 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 40 C; End T: 175 C; Start time: 5 min; CAS no: 30361285; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Hsieh, T. C. Y.; Williams, S. S.; Vejaphan, W.; Meyers, S. P., Characterization of Volatile Components of Menhaden Fish (Brevoortia tyrannus) Oil, J. Amer. Oil Chem. Soc., 66(1), 1989, 114-117., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 64 mm; Column length: 150 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 50 C; End T: 170 C; Start time: 30 min; CAS no: 30361285; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Buttery, R. G.; Kamm, J. A., Volatile components of alfalfa: possible insect host plant attractants, J. Agric. Food Chem., 28, 1980, 978-981.)NIST Spectranist ri  |

## Retention Index (Linear):

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| --- |
| 1115 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(2min) => 6C/min => 150C => 20C/min => 230C; CAS no: 30361285; Active phase: SE-54; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Schuh, C.; Schieberle, P., Characterization of the Key Aroma Compounds in the Beverage Prepared from Darjeeling Black Tea: Quantitative Differences between Tea Leaves and Infusion, J. Agric. Food Chem., 54, 2006, 916-924., 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: 240 C; CAS no: 30361285; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Baccouri, B.; Ben Temime, S.; Campeol, E.; Cioni, P. L.; Daoud, D.; Zarrouk, M., Application of solid-phase microextraction to the analysis of volatile compounds in virgin olive oils from five new cultivars, Food Chem., 102, 2007, 850-856., 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: 240 C; CAS no: 30361285; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Cioni, P. L.; Morelli, I.; Ceccarini, L.; Andolfi, L.; Macchia, M., Composition of the essential oil of Medicago marina L. from the coastal dunes of Tuscany, Italy, Flavour Fragr. J., 18, 2003, 460-462., 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: 240 C; CAS no: 30361285; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Luigi Cioni, P.; Morelli, I., Volatiles from leaves, fruits, and virgin oil from Olea europaea Cv. Olivastra Seggianese from Italy, J. Agric. Food Chem., 51, 2003, 1382-1386., 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: 220 C; Start time: 10 min; CAS no: 30361285; Active phase: HP-5; Carrier gas: N2; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Ertugrul, K.; Dural, H.; Tugay, O.; Flamini, G.; Cioni, P. L.; Morelli, I., Essential oils from flowers of Centaurea kotschyi var. kotschyi and C. kotschyi var. decumbens from Turkey, Flavour Fragr. J., 18, 2003, 95-97., 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: 220 C; Start time: 10 min; CAS no: 30361285; Active phase: HP-5; Carrier gas: N2; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Luigi Cioni, P.; Morelli, I., Essential oils of Galeopsis pubescens and G. tetrahit from Tuscany (Italy), Flavour Fragr. J., 19, 2004, 327-329., 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: 4 K/min; Start T: 40 C; End T: 260 C; End time: 10 min; Start time: 2 min; CAS no: 30361285; Active phase: DB-5; Phase thickness: 1 um; Data type: Linear RI; Authors: Methven L.; Tsoukka M.; Oruna-Concha M. J.; Parker J. K.; Mottram D. S., Influence of sulfur amino acids on the volatile and nonvolatile components of cooked salmon (Salmo salar), J. Agric. Food Chem., 55, 2007, 1427-1436.)NIST Spectranist ri  |
| 1111 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 35C (2min) => 40 C/min => 50C (1min) => 6C/min => 250C; CAS no: 30361285; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 3 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Flavor development in the ripening of anchovy (Engraulis encrasicholus L.), J. Agric. Food Chem., 43, 1995, 453-458., Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 70C(1min) => 3C/min => 80C(1min) => 5C/min => 150C => 10C/min => 280C (4min); CAS no: 30361285; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Varlet V.; Knockaert C.; Prost C.; Serot T., Comparison of odor-active volatile compounds of fresh and smoked salmon, J. Agric. Food Chem., 54, 2006, 3391-3401.)NIST Spectranist ri  |
| 1116 (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: 200 C; End time: 45 min; Start time: 5 min; CAS no: 30361285; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Whetstine M. E. C.; Drake M. A.; Nelson B. K.; Barbano D. M., Flavor profiles of full-fat and reduced-fat cheese and cheese fat made from aged cheddar with the fat removed using a novel process, J. Dairy Res., 89, 2006, 505-517.)NIST Spectranist ri  |
| 1113 (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 (2min) => 40C/min => 50C (1min) => 6C/min => 250C (10min); CAS no: 30361285; Active phase: DB-5; Carrier gas: He; Phase thickness: 1 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Changes in flavor profiles with ripening of anchovy (Engraulis encrasicholus), J. Agric. Food Chem., 43, 1995, 1883-1889., 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: 30361285; 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.)NIST Spectranist ri  |
| 1124 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Description: 40C(3min)=> 10C/min=> 60C = 3C/min => 150C => 20C/min => 250C (5min); CAS no: 30361285; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Boue, S. M.; Shih, B. Y.; Carter-Wientjes, C. H.; Cleveland, T. E., Identification of volatile compounds in soybean at various developmental stages using solid phase microextraction, J. Agric. Food Chem., 51, 2003, 4873-4876.)NIST Spectranist ri  |
| 1110 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 35C (2min) => 40 C/min => 50C (1min) => 6C/min => 250C; CAS no: 30361285; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 3 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Flavor development in the ripening of anchovy (Engraulis encrasicholus L.), J. Agric. Food Chem., 43, 1995, 453-458., Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column type: Capillary; Description: 35C (2min) => 40C/min => 50C (1min) => 6C/min => 250C (10min); CAS no: 30361285; Active phase: SE-54; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Changes in flavor profiles with ripening of anchovy (Engraulis encrasicholus), J. Agric. Food Chem., 43, 1995, 1883-1889.)NIST Spectranist ri  |
| 1596 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(2min) => 6C/min => 150C => 20C/min => 230C; CAS no: 30361285; Active phase: FFAP; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Schuh, C.; Schieberle, P., Characterization of the Key Aroma Compounds in the Beverage Prepared from Darjeeling Black Tea: Quantitative Differences between Tea Leaves and Infusion, J. Agric. Food Chem., 54, 2006, 916-924.)NIST Spectranist ri  |
| 1615 (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: 230 C; End time: 10 min; Start time: 2 min; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Mahajan, S. S.; Goddik, L.; Qian, M. C., Aroma Compounds in Sweet Whey Powder, J. Dairy Sci., 87, 2004, 4057-4063.)NIST Spectranist ri  |
| 1555 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 220 C; CAS no: 30361285; Active phase: ZB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Brunton, N. P.; Cronin, D. A.; Monahan, F. J., Volatile components associated with freshly cooked and oxidized off-flavours in turkey breast meat, Flavour Fragr. J., 17, 2002, 327-334.)NIST Spectranist ri  |
| 1605 (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: 250 C; End time: 10 min; Start time: 2 min; CAS no: 30361285; Active phase: EC-WAX; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: le Guen, S.; Prost, C.; Demaimay, M., Evaluation of the representativeness of the odor of cooked mussel extracts and the relationship between sensory descriptors and potent odorants, J. Agric. Food Chem., 49, 2001, 1321-1327., Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 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: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Le Guen, S.; Prost, C.; Demaimay, M., Characterization of odorant compounds of mussels (Mytilus edulis) according to their origin using gas chromatography-olfactometry and gas chromatography-mass spectrometry, J. Chromatogr. A, 896, 2000, 361-371.)NIST Spectranist ri  |
| 1614 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start time: 5 min; CAS no: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: le Guen, S.; Prost, C.; Demaimay, M., Critical comparison of three olfactometric methods for the identification of the most potent odorants in cooked mussels (Mytilus edulis), J. Agric. Food Chem., 48, 2000, 1307-1314.)NIST Spectranist ri  |
| 1600 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 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: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Le Guen, S.; Prost, C.; Demaimay, M., Characterization of odorant compounds of mussels (Mytilus edulis) according to their origin using gas chromatography-olfactometry and gas chromatography-mass spectrometry, J. Chromatogr. A, 896, 2000, 361-371.)NIST Spectranist ri  |
| 1588 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Description: 40C=>(6C/min)=> 80C(6min)=>(15C/min)=> 200C(10min); CAS no: 30361285; Active phase: Supelcowax-10; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Baek, H. H.; Cadwallader, K. R., Volatile compounds in flavor concentrates produced from crayfish-processing byproducts with and without protease treatment, J. Agric. Food Chem., 44, 1996, 3262-3267.)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:  | 198. 2±9. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 4±0. 4 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 43. 4±3. 0 kJ/mol  |
| Flash Point:  | 83. 0±11. 0 °C  |
| Index of Refraction:  | 1. 455  |
| Molar Refractivity:  | 39. 4±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 4  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 12  |
| ACD/LogD (pH 5. 5):  | 2. 04  |
| ACD/BCF (pH 5. 5):  | 21. 00  |
| ACD/KOC (pH 5. 5):  | 307. 64  |
| ACD/LogD (pH 7. 4):  | 2. 04  |
| ACD/BCF (pH 7. 4):  | 21. 00  |
| ACD/KOC (pH 7. 4):  | 307. 64  |
| Polar Surface Area:  | 17 Å 2  |
| Polarizability:  | 15. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 28. 0±3. 0 dyne/cm  |
| Molar Volume:  | 145. 1±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) = 2. 35Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 188. 70 (Adapted Stein & Brown method)Melting Pt (deg C): -32. 44 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 631 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 951. 7log Kow used: 2. 35 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 3943. 2 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: AldehydesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 25E-004 atm-m3/moleGroup Method: 1. 99E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 083E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 35 (KowWin est)Log Kaw used: -2. 292 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 642Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 0815Biowin2 (Non-Linear Model) : 1. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 2454 (weeks )Biowin4 (Primary Survey Model) : 4. 1343 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 8781Biowin6 (MITI Non-Linear Model): 0. 9356Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3192Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 76. 7 Pa (0. 575 mm Hg)Log Koa (Koawin est ): 4. 642Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 91E-008 Octanol/air (Koa) model: 1. 08E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 41E-006 Mackay model : 3. 13E-006 Octanol/air (Koa) model: 8. 61E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 67. 6229 E-12 cm3/molecule-secHalf-Life = 0. 158 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 898 HrsOzone Reaction: OVERALL Ozone Rate Constant = 0. 842400 E-17 cm3/molecule-secHalf-Life = 1. 360 Days (at 7E11 mol/cm3)Half-Life = 32. 650 HrsFraction sorbed to airborne particulates (phi): 2. 27E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 58. 97Log Koc: 1. 771 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 = 1. 110 (BCF = 12. 88)log Kow used: 2. 35 (estimated)Volatilization from Water: Henry LC: 1. 99E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 33. 92 hours (1. 413 days)Half-Life from Model Lake : 463. 5 hours (19. 31 days)Removal In Wastewater Treatment: Total removal: 3. 79 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 61 percentTotal to Air: 1. 08 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 413 3. 4 1000 Water 27. 9 360 1000 Soil 71. 5 720 1000 Sediment 0. 154 3. 24e+003 0 Persistence Time: 419 hr

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