

2,4-octadienal
c₈h₁₂o structure



Contents

- Retention Index (Linear):

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:**

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:**

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

20FooDBFDB008349

- Miscellaneous

- **Appearance:**

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

- Gas Chromatography

- **Retention Index (Kovats):**

1021 (estimated with error: 45)NIST

Spectramainlib_249490, replib_57735

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

1086 (Program type: Complex; Column... (show more)class: Standard no

Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary

Description: 35C(3min) => 4C/min=> 190C => 30C/min => 225C(3min)

no: 30361285; Active phase: HP-1; Phase thickness: 0. 11 um; Data type

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.*, 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 => 220C(1min); 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.; Barbano, D. M.; van Soest, P. J., Aroma compounds of some Hyblean pasture species, *Flavour Fragr. J.*, 1995, 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; Flow rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 30361285; Active phase: HP-1; Carrier gas: N2; Data type: Normal alkane RI; Authors: Tamura, H.; Nakamoto, H.; Yang, R.-H.; Sugisawa, H., Characteristic aroma compounds of 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; Flow rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 30361285; Active phase: HP-1; Carrier gas: N2; Data type: Normal alkane RI; Authors: Tamura, H.; Nakamoto, H.; Yang, R.-H.; Sugisawa, H., Characteristic aroma compounds of 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.)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: 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: 5 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, Y.; Ma, C., Aroma-active compounds of Beijing roast duck, *Flavour Fragr. J.*, 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 µm; Data type: Normal alkane RI; Authors: Buettner, A.,
selective and sensitive approach to characterize odour-active and volatile
constituents in small-scale human milk samples, *Flavour Fragr. J.*, 22, 2007,
473.)NIST Spectranist ri

1605 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat
K/min; Start T: 60 C; End T: 200 C; End time: 9.5 min; Start time: 3 min;
30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness:
µm; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintre
Strategy for the identification of key odorants: application to shrimp arom
Chromatogr. A, 1216, 2009, 6424-6432.)NIST Spectranist ri

1628 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat
K/min; Start T: 60 C; End T: 200 C; End time: 9.5 min; Start time: 3 min;
30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness:
µm; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintre
Strategy for the identification of key odorants: application to shrimp arom
Chromatogr. A, 1216, 2009, 6424-6432.)NIST Spectranist ri

1632 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat
K/min; Start T: 60 C; End T: 200 C; End time: 9.5 min; Start time: 3 min;
30361285; Active phase: DB-Wax; Carrier gas: Helium; Phase thickness:
µm; Data type: Normal alkane RI; Authors: Rochat, S.; Egger, J.; Chaintre
Strategy for the identification of key odorants: application to shrimp arom

Chromatogr. A, 1216, 2009, 6424-6432., Program type: Ramp; Column c
more)ass: Standard polar; Column diameter: 0. 53 mm; Column length: 6
Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 240 C; E
20 min; Start time: 2 min; CAS no: 30361285; Active phase: Supelcowax-
Carrier gas: He; Phase thickness: 1 um; Data type: Normal alkane RI; Aut
Rochat, S.; Chaintreau, A., Carbonyl Odorants Contributing to the In-Over
Beef Top Note, J. Agric. Food Chem., 53, 2005, 9578-9585.)NIST Spectran

1585 (Program type: Complex; Column... (show more)class: Standard po
Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capilla
Description: 40C(2min) => 40C/min => 60C(2min) => 6C/min => 180C
15C/min => 230C(10min); CAS no: 30361285; Active phase: DB-FFAP; PH
thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Buettner, A.,
selective and sensitive approach to characterize odour-active and volatil
constituents in small-scale human milk samples, Flavour Fragr. J., 22, 20
473.)NIST Spectranist ri

1601 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 210 C; CAS no: 30361285; Active phase: DB-
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI;
Kumazawa, K.; Wada, Y.; Masuda, H., Characterization of epoxydecenal i
as potent odorants in black tea (Dimbula) infusion, J. Agric. Food Chem.,
2006, 4795-4801.)NIST Spectranist ri

1630 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 53 mm; Column length: 60 m; Column type: Capillary; Heat

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: 0.25 mm; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Data type: Normal alkane RI; Authors: Rochat, S.; Chaintreau, A., Carbonell-Barral, L., 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 class: Standard polar; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 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: 0.25 mm; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Data type: Normal alkane RI; Authors: Rochat, S.; Chaintreau, A., Carbonell-Barral, L., 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 class: Standard polar; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Description: 50C(6min) => 1C/min => 130C => 10C/min => 240C (15min); CAS no: 30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0.25 mm; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Data type: Normal alkane RI; Authors: Piveteau, F.; le Guen, S.; Gandemer, B.; 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 class: Standard polar; Column diameter: 0.25 mm; Column length: 50 m; Column type: Capillary; Heat rate: 10 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., Volatile constituents of green mate and ro

mate, J. Agric. Food Chem., 39(7), 1991, 1275-1279.)NIST Spectranist ri
1590 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 175 C; Start time: 5 min; CAS no: 30361285;
phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data
Normal alkane RI; Authors: Hsieh, T. C. Y.; Williams, S. S.; Vejaphan, W.;
S. P., Characterization of Volatile Components of Menhaden Fish (Brevoo
tyrannus) Oil, J. Amer. Oil Chem. Soc., 66(1), 1989, 114-117., Program ty
Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0
Column length: 150 m; Column type: Capillary; Heat rate: 1 K/min; Start
End T: 170 C; Start time: 30 min; CAS no: 30361285; Active phase: Carbo
20M; Data type: Normal alkane RI; Authors: Buttery, R. G.; Kamm, J. A., V
components of alfalfa: possible insect host plant attractants, J. Agric. Foo
Chem., 28, 1980, 978-981.)NIST Spectranist ri

- **Retention Index (Linear):**

1115 (Program type: Complex; Column... (show more)class: Semi-standa
polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: C
Description: 40C(2min) => 6C/min => 150C => 20C/min => 230C; CAS
30361285; Active phase: SE-54; Phase thickness: 0. 25 um; Data type: LI
Authors: Schuh, C.; Schieberle, P., Characterization of the Key Aroma Cor
in the Beverage Prepared from Darjeeling Black Tea: Quantitative Differ
between Tea Leaves and Infusion, J. Agric. Food Chem., 54, 2006, 916-92
Program type: Ramp; Column cl... (show more)ass: Semi-standard non-p
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla

rate: 3 K/min; Start T: 60 C; End T: 240 C; CAS no: 30361285; Active pha
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.; Zarrou
Application of solid-phase microextraction to the analysis of volatile com
in virgin olive oils from five new cultivars, Food Chem., 102, 2007, 850-8
Program type: Ramp; Column cl... (show more)ass: Semi-standard non-p
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 3 K/min; Start T: 60 C; End T: 240 C; CAS no: 30361285; Active pha
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 d
Tuscany, Italy, Flavour Fragr. J., 18, 2003, 460-462., Program type: Ramp
Column cl... (show more)ass: Semi-standard non-polar; Column diameter
mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; St
C; End T: 240 C; CAS no: 30361285; Active phase: DB-5; Carrier gas: He;
thickness: 0. 25 um; Data type: Linear RI; Authors: Flamini, G.; Luigi Cion
Morelli, I., Volatiles from leaves, fruits, and virgin oil from *Olea europaea*
Olivastra Seggianese from Italy, J. Agric. Food Chem., 51, 2003, 1382-13
Program type: Ramp; Column cl... (show more)ass: Semi-standard non-p
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 5 K/min; Start T: 60 C; End T: 220 C; Start time: 10 min; CAS no: 30
Active phase: HP-5; Carrier gas: N2; Phase thickness: 0. 25 um; Data typ
RI; Authors: Ertugrul, K.; Dural, H.; Tugay, O.; Flamini, G.; Cioni, P. L.; Mo
Essential oils from flowers of *Centaurea kotschyi* var. *kotschyi* and *C. kot*
var. *decumbens* from Turkey, Flavour Fragr. J., 18, 2003, 95-97., Program
Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column di

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: DB-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* L. and *Salvia officinalis* L. tetrahit from Tuscany (Italy), *Flavour Fragr. J.*, 19, 2004, 327-329., Program type: Ramp; Column class: 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: 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., Effect of sulfur amino acids on the volatile and nonvolatile components of cooked salmon (*Salmo salar*), *J. Agric. Food Chem.*, 55, 2007, 1427-1436.) NIST Spectra

1111 (Program type: Complex; Column 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 (1min); CAS no: 30361285; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Flavor development during the ripening of anchovy (*Engraulis encrasicolus* L.), *J. Agric. Food Chem.*, 43, 1995, 453-458., Program type: Complex; Column class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 70C(1min) => 3C/min => 80C(1min) => 50C (1min) => 150C => 10C/min => 280C (4min); CAS no: 30361285; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: V.; Knockaert C.; Prost C.; Serot T., Comparison of odor-active volatile

compounds of fresh and smoked salmon, J. Agric. Food Chem., 54, 2006, 3401.)NIST Spectranist ri

1116 (Program type: Ramp; Column cl... (show more)ass: Semi-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: 200 C; End time: 45 min; Start time: 2 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.; B. K.; Barbano D. M., Flavor profiles of full-fat and reduced-fat cheese and fat made from aged cheddar with the fat removed using a novel process Res., 89, 2006, 505-517.)NIST Spectranist ri

1113 (Program type: Complex; Column... (show more)class: Semi-standard 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 encrasicolus*) J. Agric. Food Chem., 43, 1995, 1883-1889., Program type: Ramp; Column (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: DB-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 of mango (*Mangifera indica* L.) cultivars, J. Agric. Food Chem., 53, 2005, 22

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.; Wientjes, C. H.; Cleveland, T. E., Identification of volatile compounds in salmon 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 (10min); CAS no: 30361285; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Flavor development during the ripening of anchovy (*Engraulis encrasicolus* 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) => 40 C/min => 50C (1min) => 6C/min => 250C (10min); CAS no: 30361285; Active phase: SE-54; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Change in flavor profiles with ripening of anchovy (*Engraulis encrasicolus*), J. Agric. Food Chem., 43, 1995, 1883-1889.)NIST Spectranist ri

1596 (Program type: Complex; Column... (show more)class: 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; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: Triqui, R.; Reineccius, G. A., Change in flavor profiles with ripening of anchovy (*Engraulis encrasicolus*), J. Agric. Food Chem., 43, 1995, 1883-1889.)NIST Spectranist ri

30361285; Active phase: FFAP; Phase thickness: 0. 25 um; Data type: Lin
Authors: Schuh, C.; Schieberle, P., Characterization of the Key Aroma Comp
in the Beverage Prepared from Darjeeling Black Tea: Quantitative Differenc
between Tea Leaves and Infusion, J. Agric. Food Chem., 54, 2006, 916-92
Spectranist ri

1615 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 230 C; End time: 10 min; Start time: 2 min; C
30361285; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 5
Data type: Linear RI; Authors: Mahajan, S. S.; Goddik, L.; Qian, M. C., Aro
Compounds in Sweet Whey Powder, J. Dairy Sci., 87, 2004, 4057-4063.)N
Spectranist ri

1555 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 220 C; CAS no: 30361285; Active phase: ZB-
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors
Brunton, N. P.; Cronin, D. A.; Monahan, F. J., Volatile components associa
freshly cooked and oxidized off-flavours in turkey breast meat, Flavour F
17, 2002, 327-334.)NIST Spectranist ri

1605 (Program type: Ramp; Column cl... (show more)ass: Standard polar
diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat
K/min; Start T: 40 C; End T: 250 C; End time: 10 min; Start time: 2 min; C
30361285; Active phase: EC-WAX; Carrier gas: He; Phase thickness: 0. 5
Data type: Linear RI; Authors: le Guen, S.; Prost, C.; Demaimay, M., Evalu

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 n... 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, 361-370.)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: 4 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

1588 (Program type: Complex; Column... (show more) class: Standard pool
Column diameter: 0.25 mm; Column length: 60 m; Column type: Capillary
Description: 40C=>(6C/min)=> 80C(6min)=>(15C/min)=> 200C(10min)
no: 30361285; Active phase: Supelcowax-10; Phase thickness: 0.25 um;
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.)
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. 35
Boiling 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. 7 log Kow used: 2. 35 (estimated) no-
melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1. 01
est) = 3943. 2 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found:
Aldehydes Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1.
25E-004 atm-m³/mole Group Method: 1. 99E-005 atm-m³/mole Henrys LC [VP/WSol
estimate using EPI values]: 1. 083E-004 atm-m³/mole Log 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. 642 Log
Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN
v4. 10): Biowin1 (Linear Model) : 1. 0815 Biowin2 (Non-Linear Model) : 1.
0000 Expert 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. 8781 Biowin6
(MITI Non-Linear Model): 0. 9356 Anaerobic Biodegradation Probability: Biowin7
(Anaerobic Linear Model): 0. 3192 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): 76. 7 Pa (0. 575 mm Hg) Log Koa (Koawin est
) : 4. 642 Kp (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-sec Half-Life = 0. 158 Days (12-hr day; 1. 5E6 OH/cm³) Half-Life =
1. 898 Hrs Ozone Reaction: OVERALL Ozone Rate Constant = 0. 842400 E-17
cm³/molecule-sec Half-Life = 1. 360 Days (at 7E11 mol/cm³) Half-Life = 32. 650
Hrs Fraction sorbed to airborne particulates (phi): 2. 27E-006 (Junge,
Mackay) Note: the sorbed fraction may be resistant to atmospheric
oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 58. 97 Log 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 percent Total biodegradation: 0. 10 percent Total sludge adsorption: 2. 61
percent Total 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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