

Phenylethyl  
isovalerate c13h18o2  
structure



**ASSIGN  
BUSTER**

## Contents

- Retention Index (Linear):

Molecular Formula	$C_{13}H_{18}O_2$
Average mass	206.281 Da
Density	$1.0 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$281.9 \pm 9.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$108.0 \pm 17.1 \text{ }^\circ\text{C}$
Molar Refractivity	$60.7 \pm 0.3 \text{ cm}^3$
Polarizability	$24.1 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$34.3 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$208.6 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite
- Predicted - ChemAxon
- Predicted - Mcule

- Experimental Physico-chemical Properties

- **Experimental Boiling Point:**

- 263 °C Food and Agriculture Organization of the United Nations2-

- Phenylethyl isovalerate

- 268 °C (Literature) LabNetworkLN00227137

- 263 °C FooDBFDB013622

- **Experimental Flash Point:**

- 100

- °C LabNetworkLN00227137

- **Experimental Refraction Index:**

- 1. 482-1. 487 Food and Agriculture Organization of the United Nations2-

- Phenylethyl isovalerate

- 20 FooDBFDB013622

- Miscellaneous

- **Appearance:**

- Colourless to slighty yellow liquid; fruity or rose-like odour Food and Agric

- Organization of the United Nations2-Phenylethyl isovalerate

- Gas Chromatography

- **Retention Index (Kovats):**

- 1493 (estimated with error: 47) NIST Spectramainlib\_152550, replib\_1224

replib\_109582

1491 (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: 50 C; End T: 250 C; End time: 5 min; Start time: 5 min; CAS no: 140261; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Asuming, W. A.; Beauchamp, P. S.; Descalzo, J. T.; Dev, B. C.; Dev, V.; Frost, S.; Ma, C. W., Essential oil composition of four *Lomatium Raf.* species and their chemotaxonomy, *Biochem. Syst. Ecol.*, 33, 2005, 17-26.)NIST Spectranist ri

1490 (Program type: Ramp; Column cl... (show more)ass: Semi-standard polar; Column diameter: 0. 26 mm; Column length: 30 m; Column type: C Heat rate: 3 K/min; Start T: 60 C; End T: 246 C; CAS no: 140261; Active phase: SE-54; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Adams, Systematics of the one seeded *Juniperus* of the eastern hemisphere based on essential oils and random amplified polymorphic DNAs (RAPDs), *Biochem. Syst. Ecol.*, 28, 2000, 529-543.)NIST Spectranist ri

1955 (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: 35 C; End T: 200 C; End time: 20 min; Start time: 5 min; CAS no: 140261; Active phase: Supelcowax-10; Carrier gas: He; Data type: Kovats RI; Authors: Wong, K. C.; Teng, Y. E., Volatile Components of *Mimusops elenifolia* Flowers, *J. Essent. Oil Res.*, 6, 1994, 453-458.)NIST Spectranist ri

1961 (Program type: Ramp; Column cl... (show more)ass: Standard polar

diameter: 0.28 mm; Column length: 50 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 70 C; End T: 190 C; CAS no: 140261; Active phase: Carbowax 20M; Carrier gas: He; Data type: Kovats RI; Authors: Tressl, R.; Friese, L.; Fendesack, F.; Koppler, H., Gas chromatographic-mass spectrometric investigation of hop aroma constituents in beer, J. Agric. Food Chem., 26(1978), 1422-1426.)NIST Spectranist ri

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

1468 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar  
Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 240 C; Start time: 3 min; CAS no: 140261; Active phase: DB-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Shiota, H., New esteric components in the volatile oil of banana fruit (Musa sapientum L.), J. Agric. Food Chem., 41(11), 1993, 2062-2066., Program type: Ramp; Column cl... (show more)ass: Standard non-polar  
Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 220 C; End time: 20 min; Start time: 2 min; CAS no: 140261; Active phase: DB-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Audino, P. G.; Alzogaray, R. A.; Vassena, C.; Masuh, H.; Fontan, R.; Martinez, A.; Camps, F.; Cork, A.; Zerba, E., Volatile compounds secreted by Brindley's glands of adult Triatoma infestans: identification and biological activity of previously unidentified compounds, Journal of Vector Ecology, 32(1), 2007, 82.)NIST Spectranist ri

1486.3 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar  
Column diameter: 0.32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 70 C; End T: 190 C; CAS no: 140261; Active phase: Carbowax 20M; Carrier gas: He; Data type: Kovats RI; Authors: Tressl, R.; Friese, L.; Fendesack, F.; Koppler, H., Gas chromatographic-mass spectrometric investigation of hop aroma constituents in beer, J. Agric. Food Chem., 26(1978), 1422-1426.)NIST Spectranist ri

rate: 5 K/min; Start T: 65 C; End T: 280 C; End time: 30 min; Start time: 1  
CAS no: 140261; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickn  
um; Data type: Normal alkane RI; Authors: Joulain, D.; Casazza, A.; Laure  
Portier, D.; Guillamon, N.; Pandya, R.; Le, M.; Viljoen, A., Volatile flavor  
constituents of fruits from Southern Africa: mobola plum (Parinari curatell  
Agric. Food Chem., 52, 2004, 2322-2325.)NIST Spectranist ri

1474 (Program type: Ramp; Column cl... (show more)ass: Standard non-p  
Column type: Capillary; CAS no: 140261; Active phase: SE-30; Data type  
alkane RI; Authors: Vinogradov, B. A., Production, composition, properties  
application of essential oils, 2004.)NIST Spectranist ri

1508 (Program type: Complex; Column... (show more)class: Standard no  
Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capilla  
Description: 40C(3min) =; 5C/min =; 180C=; 15C/min =; 240C(15min); C  
140261; Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 25 um;  
type: Normal alkane RI; Authors: Nogueira, J. M. F.; Romano, A., Essentia  
from micropropagated plants of Lavandula viridis, Phytochem. Anal., 13,  
7.)NIST Spectranist ri

1459 (Program type: Ramp; Column cl... (show more)ass: Standard non-p  
Column diameter: 0. 22 mm; Column length: 50 m; Column type: Capilla  
rate: 1 K/min; Start T: 100 C; End T: 220 C; Start time: 1 min; CAS no: 14  
Active phase: OV-101; Carrier gas: He; Phase thickness: 1 um; Data type  
alkane RI; Authors: Camciuc, M.; Bessiere, J. M.; Vilarem, G.; Gaset, A., V  
components in okra seed coat, Phytochemistry, 48(2), 1998, 311-315.)N  
Spectranist ri

1457 (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: 4 K/min; Start T: 50 C; End T: 290 C; CAS no: 140261; Active phase: HP-5; Carrier gas: N2; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Bos, R.; Woerdenbag, H. J.; Hendriks, H.; Smit, H. F.; Wikstrom, M.; Scheffer, J. J. C., Composition of the essential oil from roots and rhizomes of *Valeriana wallichii* DC, *Flavour Fragr. J.*, 12, 1997, 123-131.)NIST Spectra

1465 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 240 C; Start time: 3 min; CAS no: 140261; Active phase: DB-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Shiota, H., New esteric components in the volatile oil of banana fruit (*Musa sapientum* L.), *J. Agric. Food Chem.*, 41(11), 1993, 2062.)NIST Spectra

1487 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0.32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 290 C; CAS no: 140261; Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Pavlovic, M.; Petrovic, S.; Ristic, M.; Maksimovic, Z.; Kovacevic, N., Essential oil of *Filipendula hexapetala*, *Chem. Nat. Compounds*, 43(2), 2007, 228-229.)NIST Spectra

1490 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0.32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 280 C; CAS no: 140261; Active phase: HP-5; Carrier gas: Helium; Phase thickness: 0.52 um; Data type: Normal alkane RI

RI; Authors: Pavlovic, M.; Petrovic, S.; Ristic, M.; Maksimovic, Z.; Kovacevic, M.; (2005, 228-229.)NIST Spectranist ri

1494. 7 (Program type: Ramp; Column cl... (show more)ass: Semi-standard; Column diameter: 0.32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 260 C; End time: 28 min; Start time: 0 min; CAS no: 140261; Active phase: HP-5; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Leffingwell, J. C.; Alford, E. D.; (2005, 899-915.)NIST Spectranist ri

1499 (Program type: Ramp; Column cl... (show more)ass: Semi-standard; Column diameter: 0.2 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 280 C; CAS no: 140261; Active phase: HP-5MS; Data type: Normal alkane RI; Authors: Petrakis, P. V.; Roussis, V.; Papadimitriou, D.; Vagias, C.; Tsitsimpikou, C., The effect of terpenoid exudates from 15 pine species on the feeding behavioural sequence of the late instar of the pine processionary caterpillar *Thaumetopoea pityocampa*, *Behav. Process.* 69, 2005, 303-322.)NIST Spectranist ri

1488 (Program type: Complex; Column... (show more)class: Semi-standard; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Description: 40C =; 2C/min =; 60C =; 4C/min =; 260C; CAS no: 140261; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Maia, J. G. S.; Andrade, E. H. A.; Zoghbi, M. G. B., Aromatic volatiles from two fruit varieties of jackfruit (*Artocarpus heterophyllus* La



Food Chem., 85, 2004, 195-197.)NIST Spectranist ri

1495 (Program type: Ramp; Column cl... (show more)ass: Semi-standard polar; Column type: Capillary; CAS no: 140261; Active phase: DB-5; Data Normal alkane RI; Authors: Petrakis, P. V.; Tsitsimpikou, C.; Tzakou, O.; C M.; Vagias, C.; Roussis, V., Needle volatiles from five Pinus species growi Greece, Flavour Fragr. J., 16, 2001, 249-252.)NIST Spectranist ri

1482 (Program type: Complex; Column... (show more)class: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Description: 50 0C ^ 3 K/min -; 200 0C ^ 8 K/min -; 280 0C; CAS no: 140 Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data typ Normal alkane RI; Authors: Usubillaga, A.; Aparicio, R.; Romero, M.; Rojas Khouri, N., Volatile constituents from the leaves of four Libanothamus sp from the Venezuelan Andes, Flavour Fragr. J., 16, 2001, 209-211.)NIST Spectranist ri

1983 (Program type: Ramp; Column cl... (show more)ass: Standard polar length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; E 220 C; End time: 20 min; Start time: 2 min; CAS no: 140261; Active phas Wax 52CB; Carrier gas: He; Phase thickness: 0. 32 um; Data type: Norma RI; Authors: Audino, P. G.; Alzogaray, R. A.; Vassena, C.; Masuh, H.; Fonta Gatti, P.; Martinez, A.; Camps, F.; Cork, A.; Zerba, E., Volatile compounds secreted by Brindley's glands of adult Triatoma infestans: identification a biological activity of previously unidentified compounds, Journal of Vector Ecology, 32(1), 2007, 75-82.)NIST Spectranist ri

1980 (Program type: Ramp; Column cl... (show more)ass: Standard polar  
diameter: 0. 32 mm; Column length: 15 m; Column type: Capillary; Heat  
K/min; Start T: 40 C; End T: 230 C; End time: 20 min; CAS no: 140261; Ac  
phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: N  
alkane RI; Authors: Kishimoto, T.; Wanikawa, A.; Kono, K.; Shibata, K.,  
Comparison of the Odor-Active Compounds in Unhopped Beer and Beers  
with Different Hop Varieties, J. Agric. Food Chem., 54, 2006, 8855-8861.)  
Spectranist ri

1955 (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: 200 C; End time: 30 min; Start time: 3 min; C  
140261; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness:  
um; Data type: Normal alkane RI; Authors: Wong, K. C.; Lai, F. Y., Volatile  
constituents from the fruits of four Syzygium species grown in Malaysia,  
Fragr. J., 11, 1996, 61-66., Program type: Ramp; Column cl... (show more  
Standard polar; Column type: Capillary; CAS no: 140261; Active phase: C  
20M; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production  
composition, properties and application of essential oils, 2004.)NIST Spe  
ri

1992 (Program type: Complex; Column... (show more)class: Standard po  
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla  
Description: 60 0C (10 min) ^ 10 K/min -> 220 0C (10 min) ^ 1K/min ->  
CAS no: 140261; Active phase: HP-Innowax; Carrier gas: He; Phase thickn  
25 um; Data type: Normal alkane RI; Authors: Baser, K. H. C.; Demirci, B.

Tabanca, N.; Ozek, T.; Goren, N., Composition of the essential oils of *Tanacetum armenum* (DC.) Schultz Bip., *T. balsamita* L., *T. chiliophyllum* (Fisch. & Meyer) Schultz Bip. var. *chiliophyllum* and *T. haradjani* (Rech. fil.) Grierson and the enantiomeric distribution of camphor and carvone, *Flavour Fragr. J.*, 16, 2 (1995), 195-200.)NIST Spectranist ri

1986 (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: 200 C; Start time: 2 min; CAS no: 140261; Ac phase: DB-Wax; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Umamo, 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

1927 (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: 60 C; End T: 180 C; Start time: 4 min; CAS no: 140261; Ac phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Kawakami, M.; Ganguly, S. N.; Banerjee, J.; Kobayashi, A., Aroma composition of oolong and black tea by brewed extraction method and characterizing compounds of Darjeeling tea aroma, *J. Agric. Food Chem.*, 43, 1995, 200-207.)NIST Spectranist ri

- **Retention Index (Linear):**

1463 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar Column diameter: 0.22 mm; Column length: 60 m; Column type: Capillary

rate: 2 K/min; Start T: 60 C; End T: 230 C; End time: 35 min; CAS no: 140261; Active phase: RTX-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Costa, J.; Bernardini, A., Analysis of the essential oils from aerial parts of *Eupatorium cannabinum* subsp. *corsicum* (L.) by gas chromatography with electron impact and chemical ionization mass spectrometry, *J. Chromatogr. A*, 1076, 2005, 170-178., Program type: Ramp; Column class: Standard non-polar; Column diameter: 0.25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 230 C; End time: 35 min; CAS no: 140261; Active phase: RTX-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Muselli, A.; Bernardini, A.-F.; Bighelli, A.; Casanova, J.; Costa, J., Thymol and p-cymene derivatives from essential oil of *Doronicum corsicum* L., *Flavour Fragr. J.*, 2007, 479-487.)NIST Spectranist ri

1448 (Program type: Ramp; Column class: Standard non-polar; Column diameter: 0.32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 260 C; End time: 5 min; Start time: 3 min; CAS no: 140261; Active phase: DB-1; Carrier gas: N2; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Dob T.; Berramdane T.; Chelghoum C., Analysis of the essential oil from the needles of *Pinus pinaster* growing in Algeria, *Chem. Compd. (Engl. Transl.)*, 41(5), 2005, 545-548.)NIST Spectranist ri

1466 (Program type: Ramp; Column class: Standard non-polar; Column diameter: 0.22 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 220 C; End time: 20 min; CAS no: 140261; Active phase: BP-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Costa, J.; Bernardini, A., Analysis of the essential oils from aerial parts of *Eupatorium cannabinum* subsp. *corsicum* (L.) by gas chromatography with electron impact and chemical ionization mass spectrometry, *J. Chromatogr. A*, 1076, 2005, 170-178., Program type: Ramp; Column class: Standard non-polar; Column diameter: 0.25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 60 C; End T: 230 C; End time: 35 min; CAS no: 140261; Active phase: RTX-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Muselli, A.; Bernardini, A.-F.; Bighelli, A.; Casanova, J.; Costa, J., Thymol and p-cymene derivatives from essential oil of *Doronicum corsicum* L., *Flavour Fragr. J.*, 2007, 479-487.)NIST Spectranist ri

RI; Authors: Rezzi, S.; Bighelli, A.; Mouillot, D.; Casanova, J., Composition and chemical variability of the needle essential oil of *Pinus nigra* subsp. *laricina* corsica, *Flavour Fragr. J.*, 16, 2001, 379-383.)NIST Spectranist ri

1469 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.22 mm; Column length: 25 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 70 C; End T: 295 C; CAS no: 140261; Active phase: CB; Carrier gas: N2; Data type: Linear RI; Authors: Montanarella, L.; Bos, M.; Fischer, F. C., The Essential Oil in Lamina and Petiole of *Heracleum disse* Leaves, *Planta Medica*, , 1986, 332-334.)NIST Spectranist ri

1488 (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: 280 C; Start time: 5 min; CAS no: 140261; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Saroglou, V.; Dorizas, N.; Kyriotakis, Z.; Skaltsas, A., Analysis of the essential oil composition of eight *Anthemis* species from Crete, *J. Chromatogr. A*, 1104, 2006, 313-322.)NIST Spectranist ri

1489 (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: 5 min; CAS no: 140261; Active phase: SPB-5; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Pino, J. A.; Marbot, R.; Rosado, A.; Vazquez, C., Volatile constituents of Malay rose apple [*Syzygium malaccense* (L.) Merr. & Perry], *Flavour Fragr. J.*, 19, 2004, 32-35., Program type: Ramp; Column cl... (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  
280 C; Start time: 5 min; CAS no: 140261; Active phase: HP-5MS; Carrier  
Phase thickness: 0.25 um; Data type: Linear RI; Authors: Grujic-Jovanovi  
Skaltsa, H. D.; Marin, P.; Sokovic, M., Composition and antibacterial activ  
essential oil of six *Stachys* species from Serbia, *Flavour Fragr. J.*, 19, 200  
144.)NIST Spectranist ri

1491 (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: 240 C; CAS no: 140261; Active p  
HP-5; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; A  
Macchioni, F.; Cioni, P. L.; Flamini, G.; Morelli, I.; Maccioni, S.; Ansaldi, M.  
Chemical composition of essential oils from needles, branches and cones  
*Pinus pinea*, *P. halepensis*, *P. pinaster* and *P. nigra* from central Italy, *Flavour F*  
18, 2003, 139-143.)NIST Spectranist ri

1490 (Program type: Complex; Column... (show more)class: Semi-standa  
polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: C  
Description: 50C=> 6C/min=> 100C=> 4C/min=> 280C; CAS no: 14026  
phase: HP-5; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linea  
Authors: Isidorov, V. A.; Krajewska, U.; Dubis, E. N.; Jdanova, M. A., Partit  
coefficients of alkyl aromatic hydrocarbons and esters in a hexane-aceto  
system, *J. Chromatogr. A*, 923, 2001, 127-136., Program type: Ramp; Col  
(show more)ass: Semi-standard non-polar; Column diameter: 0.25 mm;  
length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; E  
240 C; CAS no: 140261; Active phase: HP-5; Carrier gas: He; Phase thick

25 um; Data type: Linear RI; Authors: Macchioni, F.; Cioni, P. L.; Flamini, G.; Morelli, I.; Maccioni, S.; Ansaldi, M., Chemical composition of essential oil from needles, branches and cones of *Pinus pinea*, *P. halepensis*, *P. pinaster* and *P. nigra* from central Italy, *Flavour Fragr. J.*, 18, 2003, 139-143.)NIST Spectra

1954 (Program type: Ramp; Column class: (show more) Standard polar; Column diameter: 0.22 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 60 C; End T: 230 C; End time: 35 min; CAS no: 140261; Acquisition phase: RTX-Wax; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Muselli, A.; Bernardini, A.-F.; Bighelli, A.; Casanova, J.; Costa, J., Thymol derivatives from essential oil of *Doronicum corsicum* L., *Flavour Fragr. J.*, 22, 2007, 479-487.)NIST Spectra

1964 (Program type: Ramp; Column class: (show more) Standard polar; Column diameter: 0.22 mm; Column length: 60 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 60 C; End T: 230 C; End time: 35 min; CAS no: 140261; Acquisition phase: RTX-Wax; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Paolini, J.; Costa, J.; Bernardini, A., Analysis of the essential oil from aerial parts of *Eupatorium cannabinum* subsp. *corsicum* (L.) by gas chromatography with electron impact and chemical ionization mass spectrometry, *J. Chromatogr. A*, 1076, 2005, 170-178.)NIST Spectra

1980 (Program type: Ramp; Column class: (show more) Standard polar; Column diameter: 0.22 mm; Column length: 50 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 60 C; End T: 220 C; End time: 20 min; CAS no: 140261; Acquisition phase: BP-20; Carrier gas: He; Phase thickness: 0.25 um; Data type: Linear RI; Authors: Rezzi, S.; Bighelli, A.; Mouillot, D.; Casanova, J., Composition and

chemical variability of the needle essential oil of *Pinus nigra* subsp. *laricina* corsica, *Flavour Fragr. J.*, 16, 2001, 379-383.)NIST Spectranist ri

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

Density:	1. 0±0. 1 g/cm <sup>3</sup>
Boiling Point:	281. 9±9. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 6 mmHg at 25°C
Enthalpy of Vaporization:	52. 1±3. 0 kJ/mol
Flash Point:	108. 0±17. 1 °C
Index of Refraction:	1. 494
Molar Refractivity:	60. 7±0. 3 cm <sup>3</sup>
#H bond acceptors:	2
#H bond donors:	0
#Freely Rotating Bonds:	6
#Rule of 5 Violations:	0
ACD/LogP:	3. 71



ACD/LogD (pH 5. 5):	3. 92
ACD/BCF (pH 5. 5):	561. 75
ACD/KOC (pH 5. 5):	3233. 88
ACD/LogD (pH 7. 4):	3. 92
ACD/BCF (pH 7. 4):	561. 75
ACD/KOC (pH 7. 4):	3233. 88
Polar Surface Area:	26 Å <sup>2</sup>
Polarizability:	24. 1±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	34. 3±3. 0 dyne/cm
Molar Volume:	208. 6±3. 0 cm <sup>3</sup>

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 3. 97Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 275. 55 (Adapted Stein & Brown method)Melting Pt (deg C): 24. 45 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0068 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 16. 47log Kow used: 3. 97 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 13. 742 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 40E-005 atm-m3/moleGroup Method: 1. 12E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 121E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 97 (KowWin est)Log Kaw used: -2. 745 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 715Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 0063Biowin2 (Non-Linear Model) : 0. 9986Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2.

<https://assignbuster.com/phenylethyl-isovalerate-c13h18o2-structure/>

8307 (weeks )Biowin4 (Primary Survey Model) : 3. 7154 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4765Biowin6 (MITI Non-Linear Model): 0. 5722Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3542Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 944 Pa (0. 00708 mm Hg)Log Koa (Koawin est ): 6. 715Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 18E-006 Octanol/air (Koa) model: 1. 27E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000115 Mackay model : 0. 000254 Octanol/air (Koa) model: 0. 000102 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 10. 9089 E-12 cm3/mole-secHalf-Life = 0. 980 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 11. 766 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000184 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1359Log Koc: 3. 133 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 2. 078E-002 L/mol-secKb Half-Life at pH 8: 1. 057 years Kb Half-Life at pH 7: 10. 570 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 2. 358 (BCF = 228. 2)log Kow used: 3. 97 (estimated)Volatilization from Water: Henry LC: 1. 12E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 76. 55 hours (3. 189 days)Half-Life from Model Lake : 955. 5 hours (39. 81 days)Removal In Wastewater Treatment: Total removal: 29. 08 percentTotal biodegradation: 0. 31 percentTotal sludge adsorption: 28. 33 percentTotal to Air: 0. 44 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 1. 79 23. 5 1000 Water 23. 1 360 1000 Soil 72. 4 720 1000 Sediment 2. 75 3. 24e+003 0 Persistence Time: 479 hr

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