# Butanoic acid, 3-methyl-, 3,7-dimethyl-6-octenyl ester

**Other names:** Citronellyl iso-valerate
3,7-dimethyloct-6-enyl isovalerate
**Inchi:** InChI=1S/C15H28O2/c1-12(2)7-6-8-14(5)9-10-17-15(16)11-13(3)4/h7,13-14H,6,8-11H2,1
**InchiKey:** WZTNQQJXPYEGAF-UHFFFAOYSA-N
**Formula:** C15H28O2
**SMILES:** CC(C)=CCCC(C)CCOC(=O)CC(C)C
**Mol. weight [g/mol]:** 240.38
**CAS:** 68922-10-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -91.71 | kJ/mol | Joback Method |
| hf | -500.86 | kJ/mol | Joback Method |
| hfus | 29.24 | kJ/mol | Joback Method |
| hvap | 57.40 | kJ/mol | Joback Method |
| log10ws | -4.33 | | Crippen Method |
| logp | 4.348 | | Crippen Method |
| mcvol | 225.350 | ml/mol | McGowan Method |
| pc | 1551.22 | kPa | Joback Method |
| rinpol | 1563.00 | | NIST Webbook |
| rinpol | 1558.00 | | NIST Webbook |
| rinpol | 1563.00 | | NIST Webbook |
| rinpol | 1558.00 | | NIST Webbook |
| rinpol | 1563.00 | | NIST Webbook |
| ripol | 1800.00 | | NIST Webbook |
| tb | 622.05 | K | Joback Method |
| tc | 803.00 | K | Joback Method |
| tf | 281.93 | K | Joback Method |
| vc | 0.869 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 601.07 | J/mol×K | 622.05 | Joback Method |

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|---|---|---|---|---|
| cpg | 618.93 | J/mol×K | 652.21 | Joback Method |
| cpg | 635.95 | J/mol×K | 682.37 | Joback Method |
| cpg | 652.16 | J/mol×K | 712.52 | Joback Method |
| cpg | 667.59 | J/mol×K | 742.68 | Joback Method |
| cpg | 682.26 | J/mol×K | 772.84 | Joback Method |
| cpg | 696.20 | J/mol×K | 803.00 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C68922101&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |