# L-Valine, N-(3-methylbut-2-enoyl)-, isohexyl ester

**Inchi:** InChI=1S/C16H29NO3/c1-11(2)8-7-9-20-16(19)15(13(5)6)17-14(18)10-12(3)4/h10-11,13

**InchiKey:** UJOFCLKIHCMJGP-UHFFFAOYSA-N

**Formula:** C16H29NO3

**SMILES:** CC(C)=CC(=O)NC(C(=O)OCCCC(C)C)C(C)C

**Mol. weight [g/mol]:** 283.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -125.26 | kJ/mol | Joback Method |
| hf | -585.89 | kJ/mol | Joback Method |
| hfus | 35.00 | kJ/mol | Joback Method |
| hvap | 72.42 | kJ/mol | Joback Method |
| log10ws | -3.83 | | Crippen Method |
| logp | 3.073 | | Crippen Method |
| mcvol | 250.990 | ml/mol | McGowan Method |
| pc | 1536.66 | kPa | Joback Method |
| rinpol | 1934.00 | | NIST Webbook |
| rinpol | 1934.00 | | NIST Webbook |
| tb | 748.53 | K | Joback Method |
| tc | 940.66 | K | Joback Method |
| tf | 380.79 | K | Joback Method |
| vc | 0.960 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 742.04 | J/mol×K | 748.53 | Joback Method |
| cpg | 758.65 | J/mol×K | 780.55 | Joback Method |
| cpg | 774.33 | J/mol×K | 812.57 | Joback Method |
| cpg | 789.10 | J/mol×K | 844.59 | Joback Method |
| cpg | 802.99 | J/mol×K | 876.61 | Joback Method |
| cpg | 816.05 | J/mol×K | 908.64 | Joback Method |
| cpg | 828.30 | J/mol×K | 940.66 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346068&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |