# Sarcosine, n-hexanoyl-, isohexyl ester

**Inchi:** InChI=1S/C15H29NO3/c1-5-6-7-10-14(17)16(4)12-15(18)19-11-8-9-13(2)3/h13H,5-12H2
**InchiKey:** URYRQKSNOHEUEQ-UHFFFAOYSA-N
**Formula:** C15H29NO3
**SMILES:** CCCCCC(=O)N(C)CC(=O)OCCCC(C)C
**Mol. weight [g/mol]:** 271.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -179.08 | kJ/mol | Joback Method |
| hf | -648.06 | kJ/mol | Joback Method |
| hfus | 38.49 | kJ/mol | Joback Method |
| hvap | 66.54 | kJ/mol | Joback Method |
| log10ws | -3.07 | | Crippen Method |
| logp | 3.004 | | Crippen Method |
| mcvol | 241.200 | ml/mol | McGowan Method |
| pc | 1546.35 | kPa | Joback Method |
| rinpol | 1966.00 | | NIST Webbook |
| rinpol | 1966.00 | | NIST Webbook |
| tb | 684.76 | K | Joback Method |
| tc | 861.70 | K | Joback Method |
| tf | 398.37 | K | Joback Method |
| vc | 0.917 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.79 | J/mol×K | 684.76 | Joback Method |
| cpg | 705.58 | J/mol×K | 714.25 | Joback Method |
| cpg | 721.55 | J/mol×K | 743.74 | Joback Method |
| cpg | 736.70 | J/mol×K | 773.23 | Joback Method |
| cpg | 751.06 | J/mol×K | 802.72 | Joback Method |
| cpg | 764.66 | J/mol×K | 832.21 | Joback Method |
| cpg | 777.50 | J/mol×K | 861.70 | Joback Method |

# Sources

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|---|---|
| **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=U321125&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |