# Sarcosylsarcosine, N-isobutoxycarbonyl-, heptyl ester

**Inchi:** InChI=1S/C18H34N2O5/c1-6-7-8-9-10-11-24-17(22)13-19(4)16(21)12-20(5)18(23)25-14-
**InchiKey:** NABAISOCMVPTDI-UHFFFAOYSA-N
**Formula:** C18H34N2O5
**SMILES:** CCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
**Mol. weight [g/mol]:** 358.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -276.96 | kJ/mol | Joback Method |
| hf | -887.25 | kJ/mol | Joback Method |
| hfus | 52.07 | kJ/mol | Joback Method |
| hvap | 84.42 | kJ/mol | Joback Method |
| log10ws | -2.73 | | Crippen Method |
| logp | 2.683 | | Crippen Method |
| mcvol | 300.890 | ml/mol | McGowan Method |
| pc | 1287.44 | kPa | Joback Method |
| rinpol | 2423.00 | | NIST Webbook |
| tb | 842.13 | K | Joback Method |
| tc | 1033.46 | K | Joback Method |
| tf | 536.81 | K | Joback Method |
| vc | 1.127 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 957.98 | J/mol×K | 842.13 | Joback Method |
| cpg | 974.35 | J/mol×K | 874.02 | Joback Method |
| cpg | 989.63 | J/mol×K | 905.91 | Joback Method |
| cpg | 1003.85 | J/mol×K | 937.80 | Joback Method |
| cpg | 1017.03 | J/mol×K | 969.69 | Joback Method |
| cpg | 1029.20 | J/mol×K | 1001.58 | Joback Method |
| cpg | 1040.38 | J/mol×K | 1033.46 | 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=U320582&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |

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