# Sarcosine, N-(4-ethylbenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C18H27NO3/c1-5-15-8-10-16(11-9-15)18(21)19(4)13-17(20)22-12-6-7-14(2)3/h
**InchiKey:** ABDUAGNIOWPREJ-UHFFFAOYSA-N
**Formula:** C18H27NO3
**SMILES:** CCc1ccc(C(=O)N(C)CC(=O)OCCCC(C)C)cc1
**Mol. weight [g/mol]:** 305.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -51.04 | kJ/mol | Joback Method |
| hf | -484.92 | kJ/mol | Joback Method |
| hfus | 39.91 | kJ/mol | Joback Method |
| hvap | 76.16 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.300 | | Crippen Method |
| mcvol | 259.710 | ml/mol | McGowan Method |
| pc | 1580.97 | kPa | Joback Method |
| rinpol | 2361.00 | | NIST Webbook |
| tb | 785.06 | K | Joback Method |
| tc | 986.20 | K | Joback Method |
| tf | 471.12 | K | Joback Method |
| vc | 0.978 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 774.39 | J/mol×K | 785.06 | Joback Method |
| cpg | 790.71 | J/mol×K | 818.58 | Joback Method |
| cpg | 805.97 | J/mol×K | 852.11 | Joback Method |
| cpg | 820.20 | J/mol×K | 885.63 | Joback Method |
| cpg | 833.44 | J/mol×K | 919.16 | Joback Method |
| cpg | 845.72 | J/mol×K | 952.68 | Joback Method |
| cpg | 857.09 | J/mol×K | 986.20 | 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=U321232&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 |