# Sarcosine, N-(4-methylbenzoyl)-, isobutyl ester

**Inchi:** InChI=1S/C15H21NO3/c1-11(2)10-19-14(17)9-16(4)15(18)13-7-5-12(3)6-8-13/h5-8,11H,
**InchiKey:** IHAMTAGWELIWOU-UHFFFAOYSA-N
**Formula:** C15H21NO3
**SMILES:** Cc1ccc(C(=O)N(C)CC(=O)OCC(C)C)cc1
**Mol. weight [g/mol]:** 263.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -76.30 | kJ/mol | Joback Method |
| hf | -423.00 | kJ/mol | Joback Method |
| hfus | 32.14 | kJ/mol | Joback Method |
| hvap | 69.48 | kJ/mol | Joback Method |
| log10ws | -2.80 | | Crippen Method |
| logp | 2.266 | | Crippen Method |
| mcvol | 217.440 | ml/mol | McGowan Method |
| pc | 2016.32 | kPa | Joback Method |
| rinpol | 2066.00 | | NIST Webbook |
| rinpol | 2066.00 | | NIST Webbook |
| tb | 716.42 | K | Joback Method |
| tc | 922.64 | K | Joback Method |
| tf | 437.31 | K | Joback Method |
| vc | 0.809 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 606.64 | J/mol×K | 716.42 | Joback Method |
| cpg | 622.19 | J/mol×K | 750.79 | Joback Method |
| cpg | 636.72 | J/mol×K | 785.16 | Joback Method |
| cpg | 650.28 | J/mol×K | 819.53 | Joback Method |
| cpg | 662.89 | J/mol×K | 853.90 | Joback Method |
| cpg | 674.60 | J/mol×K | 888.27 | Joback Method |
| cpg | 685.42 | J/mol×K | 922.64 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321214&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 |

# 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 |