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

**Inchi:** InChI=1S/C14H18ClNO3/c1-10(2)9-19-13(17)8-16(3)14(18)11-4-6-12(15)7-5-11/h4-7,10
**InchiKey:** BIRRTJZKUPXLRD-UHFFFAOYSA-N
**Formula:** C14H18ClNO3
**SMILES:** CC(C)COC(=O)CN(C)C(=O)c1ccc(Cl)cc1
**Mol. weight [g/mol]:** 283.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -96.65 | kJ/mol | Joback Method |
| hf | -418.10 | kJ/mol | Joback Method |
| hfus | 33.75 | kJ/mol | Joback Method |
| hvap | 71.64 | kJ/mol | Joback Method |
| log10ws | -3.01 | | Crippen Method |
| logp | 2.611 | | Crippen Method |
| mcvol | 215.590 | ml/mol | McGowan Method |
| pc | 2127.56 | kPa | Joback Method |
| rinpol | 2117.00 | | NIST Webbook |
| rinpol | 2117.00 | | NIST Webbook |
| tb | 730.97 | K | Joback Method |
| tc | 943.15 | K | Joback Method |
| tf | 455.96 | K | Joback Method |
| vc | 0.802 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 579.70 | J/mol×K | 730.97 | Joback Method |
| cpg | 593.74 | J/mol×K | 766.33 | Joback Method |
| cpg | 606.80 | J/mol×K | 801.70 | Joback Method |
| cpg | 618.91 | J/mol×K | 837.06 | Joback Method |
| cpg | 630.10 | J/mol×K | 872.43 | Joback Method |
| cpg | 640.41 | J/mol×K | 907.79 | Joback Method |
| cpg | 649.88 | J/mol×K | 943.15 | Joback Method |

# Sources

| | |
|---|---|
| **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=U321348&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |