

# Sarcosine, N-(3-phenylpropionyl)-, ethyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C14H19NO3/c1-3-18-14(17)11-15(2)13(16)10-9-12-7-5-4-6-8-12/h4-8H,3,9-11 |
| <b>InchiKey:</b>            | QH FYQHMIIFHSDB-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H19NO3  |
| <b>SMILES:</b>              | CCOC(=O)CN(C)C(=O)CCc1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 249.31   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -72.65  | kJ/mol               | Joback Method  |
| hf            | -385.61 | kJ/mol               | Joback Method  |
| hfus          | 33.46   | kJ/mol               | Joback Method  |
| hvap          | 66.98   | kJ/mol               | Joback Method  |
| log10ws       | -1.99   |                      | Crippen Method |
| logp          | 1.641   |                      | Crippen Method |
| mvol          | 203.350 | ml/mol               | McGowan Method |
| pc            | 2216.62 | kPa                  | Joback Method  |
| rinpol        | 2020.00 |                      | NIST Webbook   |
| tb            | 689.00  | K                    | Joback Method  |
| tc            | 893.48  | K                    | Joback Method  |
| tf            | 428.52  | K                    | Joback Method  |
| vc            | 0.759   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 553.17 | J/mol×K | 689.00          | Joback Method |
| cpg           | 568.23 | J/mol×K | 723.08          | Joback Method |
| cpg           | 582.32 | J/mol×K | 757.16          | Joback Method |
| cpg           | 595.47 | J/mol×K | 791.24          | Joback Method |
| cpg           | 607.72 | J/mol×K | 825.32          | Joback Method |
| cpg           | 619.10 | J/mol×K | 859.40          | Joback Method |
| cpg           | 629.65 | J/mol×K | 893.48          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321410&amp;Units=SI</a> |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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