

# Sarcosine, N-(cyclohexylcarbonyl)-, nonyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C19H35NO3/c1-3-4-5-6-7-8-12-15-23-18(21)16-20(2)19(22)17-13-10-9-11-14- |
| InchiKey:            | UMGABMVHSIHMLJ-UHFFFAOYSA-N  |
| Formula:             | C19H35NO3  |
| SMILES:              | CCCCCCCCCOC(=O)CN(C)C(=O)C1CCCCC1  |
| Mol. weight [g/mol]: | 325.49   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -118.51 | kJ/mol               | Joback Method  |
| hf            | -671.02 | kJ/mol               | Joback Method  |
| hfus          | 44.21   | kJ/mol               | Joback Method  |
| hvap          | 76.26   | kJ/mol               | Joback Method  |
| log10ws       | -4.64   |                      | Crippen Method |
| logp          | 4.319   |                      | Crippen Method |
| mvol          | 286.700 | ml/mol               | McGowan Method |
| pc            | 1341.76 | kPa                  | Joback Method  |
| rinpol        | 2463.00 |                      | NIST Webbook   |
| rinpol        | 2463.00 |                      | NIST Webbook   |
| tb            | 796.27  | K                    | Joback Method  |
| tc            | 990.15  | K                    | Joback Method  |
| tf            | 465.83  | K                    | Joback Method  |
| vc            | 1.081   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 917.34  | J/mol×K | 796.27          | Joback Method |
| cpg           | 936.59  | J/mol×K | 828.58          | Joback Method |
| cpg           | 954.62  | J/mol×K | 860.90          | Joback Method |
| cpg           | 971.47  | J/mol×K | 893.21          | Joback Method |
| cpg           | 987.17  | J/mol×K | 925.52          | Joback Method |
| cpg           | 1001.76 | J/mol×K | 957.83          | Joback Method |
| cpg           | 1015.28 | J/mol×K | 990.15          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U321535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321535&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>hvp:</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>rinp:</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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