

# Sarcosine, N-(4-butylbenzoyl)-, heptyl ester

Inchi:

AVXGHNOKRAVJDF-UHFFFAOYSA-N

InchiKey:

C21H33NO3

Formula:

CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(CCCC)cc1

SMILES:

347.49

Mol. weight [g/mol]:

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -23.34  | kJ/mol  | Joback Method  |
| hf            | -541.56 | kJ/mol  | Joback Method  |
| hfus          | 51.20   | kJ/mol  | Joback Method  |
| hvap          | 83.22   | kJ/mol  | Joback Method  |
| log10ws       | -5.47   |         | Crippen Method |
| logp          | 4.615   |         | Crippen Method |
| mcvol         | 301.980 | ml/mol  | McGowan Method |
| pc            | 1265.55 | kPa     | Joback Method  |
| rinpol        | 2698.00 |         | NIST Webbook   |
| rinpol        | 2698.00 |         | NIST Webbook   |
| tb            | 854.14  | K       | Joback Method  |
| tc            | 1053.99 | K       | Joback Method  |
| tf            | 519.93  | K       | Joback Method  |
| vc            | 1.151   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 950.02  | J/mol×K | 854.14          | Joback Method |
| cpg           | 966.86  | J/mol×K | 887.45          | Joback Method |
| cpg           | 982.58  | J/mol×K | 920.76          | Joback Method |
| cpg           | 997.22  | J/mol×K | 954.06          | Joback Method |
| cpg           | 1010.84 | J/mol×K | 987.37          | Joback Method |
| cpg           | 1023.47 | J/mol×K | 1020.68         | Joback Method |
| cpg           | 1035.16 | J/mol×K | 1053.99         | 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.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=U321136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321136&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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