

# Sarcosine, n-pentafluorobenzoyl-, nonyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C19H24F5NO3/c1-3-4-5-6-7-8-9-10-28-12(26)11-25(2)19(27)13-14(20)16(22)1 |
| <b>InchiKey:</b>            | WECVDIZBVLYKKH-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H24F5NO3  |
| <b>SMILES:</b>              | CCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F                                   |
| <b>Mol. weight [g/mol]:</b> | 409.39   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -1052.75 | kJ/mol               | Joback Method  |
| hf            | -1526.71 | kJ/mol               | Joback Method  |
| hfus          | 59.87    | kJ/mol               | Joback Method  |
| hvap          | 77.33    | kJ/mol               | Joback Method  |
| log10ws       | -6.32    |                      | Crippen Method |
| logp          | 4.748    |                      | Crippen Method |
| mcvol         | 282.650  | ml/mol               | McGowan Method |
| pc            | 1185.79  | kPa                  | Joback Method  |
| rinsol        | 2261.00  |                      | NIST Webbook   |
| tb            | 824.65   | K                    | Joback Method  |
| tc            | 1010.97  | K                    | Joback Method  |
| tf            | 550.42   | K                    | Joback Method  |
| vc            | 1.129    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 866.39 | J/mol×K | 824.65          | Joback Method |
| cpg           | 880.74 | J/mol×K | 855.70          | Joback Method |
| cpg           | 894.18 | J/mol×K | 886.76          | Joback Method |
| cpg           | 906.72 | J/mol×K | 917.81          | Joback Method |
| cpg           | 918.39 | J/mol×K | 948.86          | Joback Method |
| cpg           | 929.20 | J/mol×K | 979.91          | Joback Method |
| cpg           | 939.18 | J/mol×K | 1010.97         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U321550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321550&amp;Units=SI</a> |
| <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>                         |

# 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>hvac:</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>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</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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