

# 2,5-Difluorobenzamide, N,N-dihexyl-

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H29F2NO/c1-3-5-7-9-13-22(14-10-8-6-4-2)19(23)17-15-16(20)11-12-18(17) |
| <b>InchiKey:</b>            | MVYGYAQUBJNSQZ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C19H29F2NO  |
| <b>SMILES:</b>              | CCCCCN(CCCCC)C(=O)c1cc(F)ccc1F  |
| <b>Mol. weight [g/mol]:</b> | 325.44  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -205.51 | kJ/mol               | Joback Method  |
| hf            | -659.17 | kJ/mol               | Joback Method  |
| hfus          | 49.01   | kJ/mol               | Joback Method  |
| hvap          | 68.64   | kJ/mol               | Joback Method  |
| log10ws       | -6.46   |                      | Crippen Method |
| logp          | 5.568   |                      | Crippen Method |
| mvol          | 269.900 | ml/mol               | McGowan Method |
| pc            | 1303.29 | kPa                  | Joback Method  |
| rinpol        | 2158.00 |                      | NIST Webbook   |
| tb            | 735.61  | K                    | Joback Method  |
| tc            | 916.95  | K                    | Joback Method  |
| tf            | 438.93  | K                    | Joback Method  |
| vc            | 1.052   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 794.39 | J/mol×K | 735.61          | Joback Method |
| cpg           | 811.55 | J/mol×K | 765.83          | Joback Method |
| cpg           | 827.78 | J/mol×K | 796.06          | Joback Method |
| cpg           | 843.14 | J/mol×K | 826.28          | Joback Method |
| cpg           | 857.64 | J/mol×K | 856.50          | Joback Method |
| cpg           | 871.34 | J/mol×K | 886.72          | Joback Method |
| cpg           | 884.27 | J/mol×K | 916.95          | 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=U358046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358046&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>mccol:</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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