

# D-Alanine, N-(2,4-difluorobenzoyl)-, octadecyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C28H45F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-34-28(33)23 |
| InchiKey:            | HEGHNNRSYXWJPO-UHFFFAOYSA-N   |
| Formula:             | C28H45F2NO3   |
| SMILES:              | CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F                                   |
| Mol. weight [g/mol]: | 481.66  |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -387.48  | kJ/mol               | Joback Method  |
| hf            | -1109.07 | kJ/mol               | Joback Method  |
| hfus          | 73.66    | kJ/mol               | Joback Method  |
| hvap          | 101.84   | kJ/mol               | Joback Method  |
| log10ws       | -9.83    |                      | Crippen Method |
| logp          | 7.888    |                      | Crippen Method |
| mvol          | 404.150  | ml/mol               | McGowan Method |
| pc            | 786.83   | kPa                  | Joback Method  |
| rinpol        | 3295.00  |                      | NIST Webbook   |
| tb            | 1055.11  | K                    | Joback Method  |
| tc            | 1306.31  | K                    | Joback Method  |
| tf            | 617.71   | K                    | Joback Method  |
| vc            | 1.591    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1414.55 | J/molxK | 1055.11         | Joback Method |
| cpg           | 1432.93 | J/molxK | 1096.98         | Joback Method |
| cpg           | 1449.47 | J/molxK | 1138.84         | Joback Method |
| cpg           | 1464.29 | J/molxK | 1180.71         | Joback Method |
| cpg           | 1477.50 | J/molxK | 1222.57         | Joback Method |
| cpg           | 1489.19 | J/molxK | 1264.44         | Joback Method |
| cpg           | 1499.48 | J/molxK | 1306.31         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U348463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348463&amp;Units=SI</a> |
| <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>                                     |

# 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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