

# D-Alanine, N-(3,4-difluorobenzoyl)-, pentadecyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C25H39F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-31-25(30)20(2)28-24(2) |
| <b>InchiKey:</b>            | KEYUFLIXDIBWST-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C25H39F2NO3   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1                                    |
| <b>Mol. weight [g/mol]:</b> | 439.58  |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -412.74  | kJ/mol               | Joback Method  |
| hf            | -1047.15 | kJ/mol               | Joback Method  |
| hfus          | 65.89    | kJ/mol               | Joback Method  |
| hvap          | 95.16    | kJ/mol               | Joback Method  |
| log10ws       | -8.57    |                      | Crippen Method |
| logp          | 6.718    |                      | Crippen Method |
| mvol          | 361.880  | ml/mol               | McGowan Method |
| pc            | 931.21   | kPa                  | Joback Method  |
| rinpol        | 3040.00  |                      | NIST Webbook   |
| rinpol        | 3040.00  |                      | NIST Webbook   |
| tb            | 986.47   | K                    | Joback Method  |
| tc            | 1209.93  | K                    | Joback Method  |
| tf            | 583.90   | K                    | Joback Method  |
| vc            | 1.423    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1226.29 | J/mol×K | 986.47          | Joback Method |
| cpg           | 1243.20 | J/mol×K | 1023.71         | Joback Method |
| cpg           | 1258.65 | J/mol×K | 1060.96         | Joback Method |
| cpg           | 1272.72 | J/mol×K | 1098.20         | Joback Method |
| cpg           | 1285.46 | J/mol×K | 1135.45         | Joback Method |
| cpg           | 1296.95 | J/mol×K | 1172.69         | Joback Method |
| cpg           | 1307.25 | J/mol×K | 1209.93         | 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=U348370&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348370&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rlnol:</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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