

# 2,5-Difluorobenzoic acid, 4-dodecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H28F2O2/c1-3-5-6-7-8-9-11-16(10-4-2)23-19(22)17-14-15(20)12-13-18(17)

BVFKMVXWYWNYHB-UHFFFAOYSA-N

C19H28F2O2

CCCCCCCCC(CCC)OC(=O)c1cc(F)ccc1F

326.42

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -423.73 | kJ/mol  | Joback Method  |
| hf            | -864.20 | kJ/mol  | Joback Method  |
| hfus          | 43.65   | kJ/mol  | Joback Method  |
| hvap          | 68.62   | kJ/mol  | Joback Method  |
| log10ws       | -7.09   |         | Crippen Method |
| logp          | 6.041   |         | Crippen Method |
| mcvol         | 265.790 | ml/mol  | McGowan Method |
| pc            | 1296.73 | kPa     | Joback Method  |
| rinpol        | 2017.00 |         | NIST Webbook   |
| rinpol        | 2017.00 |         | NIST Webbook   |
| tb            | 745.15  | K       | Joback Method  |
| tc            | 929.57  | K       | Joback Method  |
| tf            | 413.69  | K       | Joback Method  |
| vc            | 1.046   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 783.42 | J/mol×K | 745.15          | Joback Method |
| cpg           | 800.35 | J/mol×K | 775.89          | Joback Method |
| cpg           | 816.35 | J/mol×K | 806.62          | Joback Method |
| cpg           | 831.44 | J/mol×K | 837.36          | Joback Method |
| cpg           | 845.65 | J/mol×K | 868.10          | Joback Method |
| cpg           | 859.00 | J/mol×K | 898.84          | Joback Method |
| cpg           | 871.51 | J/mol×K | 929.57          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U338471&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338471&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>                                 |

# 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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