

# 2,5-Difluorobenzoic acid, 7-pentadecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C22H34F2O2/c1-3-5-7-9-10-12-14-19(13-11-8-6-4-2)26-22(25)20-17-18(23)15

KISZVKMOJNIQGQ-UHFFFAOYSA-N

C22H34F2O2

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

368.50

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -398.47 | kJ/mol  | Joback Method  |
| hf            | -926.12 | kJ/mol  | Joback Method  |
| hfus          | 51.42   | kJ/mol  | Joback Method  |
| hvap          | 75.30   | kJ/mol  | Joback Method  |
| log10ws       | -8.35   |         | Crippen Method |
| logp          | 7.211   |         | Crippen Method |
| mcvol         | 308.060 | ml/mol  | McGowan Method |
| pc            | 1064.48 | kPa     | Joback Method  |
| rinpol        | 2285.00 |         | NIST Webbook   |
| rinpol        | 2285.00 |         | NIST Webbook   |
| tb            | 813.79  | K       | Joback Method  |
| tc            | 1001.75 | K       | Joback Method  |
| tf            | 447.50  | K       | Joback Method  |
| vc            | 1.214   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 960.31  | J/mol×K | 813.79          | Joback Method |
| cpg           | 978.23  | J/mol×K | 845.12          | Joback Method |
| cpg           | 995.09  | J/mol×K | 876.44          | Joback Method |
| cpg           | 1010.93 | J/mol×K | 907.77          | Joback Method |
| cpg           | 1025.77 | J/mol×K | 939.09          | Joback Method |
| cpg           | 1039.66 | J/mol×K | 970.42          | Joback Method |
| cpg           | 1052.62 | J/mol×K | 1001.75         | 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=U338488&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338488&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>                         |
| <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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