

# 5-Fluoro-2-trifluoromethylbenzoic acid, 4-dodecyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C20H28F4O2/c1-3-5-6-7-8-9-11-16(10-4-2)26-19(25)17-14-15(21)12-13-18(17) |
| <b>InchiKey:</b>            | TUTBSGDMRDVHTH-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C20H28F4O2  |
| <b>SMILES:</b>              | CCCCCCCCC(CCC)OC(=O)c1cc(F)ccc1C(F)(F)F   |
| <b>Mol. weight [g/mol]:</b> | 376.43  |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -802.09  | kJ/mol               | Joback Method  |
| hf            | -1285.81 | kJ/mol               | Joback Method  |
| hfus          | 44.99    | kJ/mol               | Joback Method  |
| hvap          | 67.92    | kJ/mol               | Joback Method  |
| log10ws       | -7.87    |                      | Crippen Method |
| logp          | 6.921    |                      | Crippen Method |
| mcvol         | 283.420  | ml/mol               | McGowan Method |
| pc            | 1153.78  | kPa                  | Joback Method  |
| rinpol        | 1970.00  |                      | NIST Webbook   |
| rinpol        | 1970.00  |                      | NIST Webbook   |
| tb            | 763.34   | K                    | Joback Method  |
| tc            | 944.85   | K                    | Joback Method  |
| tf            | 428.56   | K                    | Joback Method  |
| vc            | 1.127    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 858.25 | J/mol×K | 763.34          | Joback Method |
| cpg           | 874.80 | J/mol×K | 793.59          | Joback Method |
| cpg           | 890.39 | J/mol×K | 823.84          | Joback Method |
| cpg           | 905.08 | J/mol×K | 854.10          | Joback Method |
| cpg           | 918.89 | J/mol×K | 884.35          | Joback Method |
| cpg           | 931.87 | J/mol×K | 914.60          | Joback Method |
| cpg           | 944.06 | J/mol×K | 944.85          | 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=U338546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338546&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>h vap:</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>r in pol:</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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