

# 4-Fluoro-3-trifluoromethylbenzoic acid, 3-tetradecyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C22H32F4O2/c1-3-5-6-7-8-9-10-11-12-13-18(4-2)28-21(27)17-14-15-20(23)19 |
| InchiKey:            | DBKHJBRCBXMWAI-UHFFFAOYSA-N  |
| Formula:             | C22H32F4O2   |
| SMILES:              | CCCCCCCCCCCC(CC)OC(=O)c1ccc(F)c(C(F)(F)F)c1                                      |
| Mol. weight [g/mol]: | 404.48   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -785.25  | kJ/mol               | Joback Method  |
| hf            | -1327.09 | kJ/mol               | Joback Method  |
| hfus          | 50.17    | kJ/mol               | Joback Method  |
| hvap          | 72.37    | kJ/mol               | Joback Method  |
| log10ws       | -8.70    |                      | Crippen Method |
| logp          | 7.701    |                      | Crippen Method |
| mcvol         | 311.600  | ml/mol               | McGowan Method |
| pc            | 1016.83  | kPa                  | Joback Method  |
| rinpol        | 2197.00  |                      | NIST Webbook   |
| rinpol        | 2197.00  |                      | NIST Webbook   |
| tb            | 809.10   | K                    | Joback Method  |
| tc            | 994.47   | K                    | Joback Method  |
| tf            | 451.10   | K                    | Joback Method  |
| vc            | 1.238    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 976.20  | J/mol×K | 809.10          | Joback Method |
| cpg           | 993.46  | J/mol×K | 839.99          | Joback Method |
| cpg           | 1009.71 | J/mol×K | 870.89          | Joback Method |
| cpg           | 1024.97 | J/mol×K | 901.78          | Joback Method |
| cpg           | 1039.30 | J/mol×K | 932.68          | Joback Method |
| cpg           | 1052.75 | J/mol×K | 963.57          | Joback Method |
| cpg           | 1065.36 | J/mol×K | 994.47          | 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=U338684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338684&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>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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