# 6-Fluoro-2-trifluoromethylbenzoic acid, decyl ester

**Inchi:** InChI=1S/C18H24F4O2/c1-2-3-4-5-6-7-8-9-13-24-17(23)16-14(18(20,21)22)11-10-12-15

**InchiKey:** AZJKCFVBWBWZNX-UHFFFAOYSA-N

**Formula:** C18H24F4O2

**SMILES:** CCCCCCCCCCOC(=O)c1c(F)cccc1C(F)(F)F

**Mol. weight [g/mol]:** 348.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -816.49 | kJ/mol | Joback Method |
| hf | -1239.25 | kJ/mol | Joback Method |
| hfus | 43.33 | kJ/mol | Joback Method |
| hvap | 63.85 | kJ/mol | Joback Method |
| log10ws | -6.92 | | Crippen Method |
| logp | 6.142 | | Crippen Method |
| mcvol | 255.240 | ml/mol | McGowan Method |
| pc | 1312.75 | kPa | Joback Method |
| rinpol | 1937.00 | | NIST Webbook |
| rinpol | 1937.00 | | NIST Webbook |
| tb | 718.02 | K | Joback Method |
| tc | 896.17 | K | Joback Method |
| tf | 421.02 | K | Joback Method |
| vc | 1.020 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 743.55 | J/mol×K | 718.02 | Joback Method |
| cpg | 759.20 | J/mol×K | 747.71 | Joback Method |
| cpg | 774.00 | J/mol×K | 777.40 | Joback Method |
| cpg | 787.96 | J/mol×K | 807.10 | Joback Method |
| cpg | 801.12 | J/mol×K | 836.79 | Joback Method |
| cpg | 813.51 | J/mol×K | 866.48 | Joback Method |
| cpg | 825.17 | J/mol×K | 896.17 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338984&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |