# 2,5-Di(trifluoromethyl)benzoic acid, heptyl ester

**Inchi:** InChI=1S/C16H18F6O2/c1-2-3-4-5-6-9-24-14(23)12-10-11(15(17,18)19)7-8-13(12)16(20

**InchiKey:** JCOLHBBBQMNISZ-UHFFFAOYSA-N

**Formula:** C16H18F6O2

**SMILES:** CCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

**Mol. weight [g/mol]:** 356.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1220.11 | kJ/mol | Joback Method |
| hf | -1598.94 | kJ/mol | Joback Method |
| hfus | 36.90 | kJ/mol | Joback Method |
| hvap | 56.47 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 5.851 | | Crippen Method |
| mcvol | 230.600 | ml/mol | McGowan Method |
| pc | 1435.89 | kPa | Joback Method |
| rinpol | 1555.00 | | NIST Webbook |
| rinpol | 1555.00 | | NIST Webbook |
| tb | 667.57 | K | Joback Method |
| tc | 841.31 | K | Joback Method |
| tf | 402.08 | K | Joback Method |
| vc | 0.933 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 652.24 | J/mol×K | 667.57 | Joback Method |
| cpg | 666.46 | J/mol×K | 696.53 | Joback Method |
| cpg | 679.86 | J/mol×K | 725.48 | Joback Method |
| cpg | 692.46 | J/mol×K | 754.44 | Joback Method |
| cpg | 704.32 | J/mol×K | 783.40 | Joback Method |
| cpg | 715.46 | J/mol×K | 812.35 | Joback Method |
| cpg | 725.93 | J/mol×K | 841.31 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338940&Units=SI |

# 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 |