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

**Inchi:** InChI=1S/C15H14F6O2/c16-14(17,18)9-6-7-12(15(19,20)21)11(8-9)13(22)23-10-4-2-1-3-

**InchiKey:** UQTDQXGUPGUFQM-UHFFFAOYSA-N

**Formula:** C15H14F6O2

**SMILES:** O=C(OC1CCCCC1)c1cc(C(F)(F)F)ccc1C(F)(F)F

**Mol. weight [g/mol]:** 340.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1204.08 | kJ/mol | Joback Method |
| hf | -1523.98 | kJ/mol | Joback Method |
| hfus | 26.14 | kJ/mol | Joback Method |
| hvap | 54.67 | kJ/mol | Joback Method |
| log10ws | -6.02 | | Crippen Method |
| logp | 5.214 | | Crippen Method |
| mcvol | 205.650 | ml/mol | McGowan Method |
| pc | 1829.41 | kPa | Joback Method |
| rinpol | 1525.00 | | NIST Webbook |
| rinpol | 1525.00 | | NIST Webbook |
| tb | 664.24 | K | Joback Method |
| tc | 863.45 | K | Joback Method |
| tf | 398.19 | K | Joback Method |
| vc | 0.810 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 591.43 | J/mol×K | 664.24 | Joback Method |
| cpg | 607.37 | J/mol×K | 697.44 | Joback Method |
| cpg | 622.16 | J/mol×K | 730.64 | Joback Method |
| cpg | 635.84 | J/mol×K | 763.85 | Joback Method |
| cpg | 648.48 | J/mol×K | 797.05 | Joback Method |
| cpg | 660.14 | J/mol×K | 830.25 | Joback Method |
| cpg | 670.87 | J/mol×K | 863.45 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357740&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

| | |
|---|---|
| **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 |

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