# Succinic acid, 2,2-dichloroethyl 2-fluoro-3-(trifluoromethyl)phenyl ester

**Inchi:** InChI=1S/C13H10Cl2F4O4/c14-9(15)6-22-10(20)4-5-11(21)23-8-3-1-2-7(12(8)16)13(17,1

**InchiKey:** LZBXMPWNKXXAIC-UHFFFAOYSA-N

**Formula:** C13H10Cl2F4O4

**SMILES:** O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC(Cl)Cl

**Mol. weight [g/mol]:** 377.12

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1118.81 | kJ/mol | Joback Method |
| hf | -1417.61 | kJ/mol | Joback Method |
| hfus | 38.04 | kJ/mol | Joback Method |
| hvap | 70.26 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 3.877 | | Crippen Method |
| mcvol | 216.710 | ml/mol | McGowan Method |
| pc | 1890.36 | kPa | Joback Method |
| rinpol | 1978.00 | | NIST Webbook |
| rinpol | 1978.00 | | NIST Webbook |
| tb | 754.33 | K | Joback Method |
| tc | 953.47 | K | Joback Method |
| tf | 481.67 | K | Joback Method |
| vc | 0.857 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 569.78 | J/mol×K | 754.33 | Joback Method |
| cpg | 579.94 | J/mol×K | 787.52 | Joback Method |
| cpg | 589.32 | J/mol×K | 820.71 | Joback Method |
| cpg | 597.93 | J/mol×K | 853.90 | Joback Method |
| cpg | 605.79 | J/mol×K | 887.09 | Joback Method |
| cpg | 612.93 | J/mol×K | 920.28 | Joback Method |
| cpg | 619.37 | J/mol×K | 953.47 | Joback Method |

# Sources

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|---|---|
| **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=U390782&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |