# Succinic acid, 1,1,1-trifluoroprop-2-yl 2-chloro-4-methylphenyl ester

**Inchi:** InChI=1S/C14H14ClF3O4/c1-8-3-4-11(10(15)7-8)22-13(20)6-5-12(19)21-9(2)14(16,17)18

**InchiKey:** GXDCKHCFHBUYTJ-UHFFFAOYSA-N

**Formula:** C14H14ClF3O4

**SMILES:** Cc1ccc(OC(=O)CCC(=O)OC(C)C(F)(F)F)c(Cl)c1

**Mol. weight [g/mol]:** 338.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -903.65 | kJ/mol | Joback Method |
| hf | -1226.40 | kJ/mol | Joback Method |
| hfus | 33.35 | kJ/mol | Joback Method |
| hvap | 68.92 | kJ/mol | Joback Method |
| log10ws | -4.68 | | Crippen Method |
| logp | 3.828 | | Crippen Method |
| mcvol | 216.790 | ml/mol | McGowan Method |
| pc | 1867.55 | kPa | Joback Method |
| rinpol | 1825.00 | | NIST Webbook |
| rinpol | 1825.00 | | NIST Webbook |
| tb | 740.51 | K | Joback Method |
| tc | 940.87 | K | Joback Method |
| tf | 462.43 | K | Joback Method |
| vc | 0.846 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 591.27 | J/mol×K | 740.51 | Joback Method |
| cpg | 603.34 | J/mol×K | 773.90 | Joback Method |
| cpg | 614.55 | J/mol×K | 807.30 | Joback Method |
| cpg | 624.92 | J/mol×K | 840.69 | Joback Method |
| cpg | 634.47 | J/mol×K | 874.08 | Joback Method |
| cpg | 643.22 | J/mol×K | 907.47 | Joback Method |
| cpg | 651.21 | J/mol×K | 940.87 | Joback Method |

# Sources

| | |
|---|---|
| **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=U390208&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 |