# Succinic acid, 3-chlorophenyl 2,2,3,3,3-pentafluoropropyl ester

**Inchi:** InChI=1S/C13H10ClF5O4/c14-8-2-1-3-9(6-8)23-11(21)5-4-10(20)22-7-12(15,16)13(17,18

**InchiKey:** IFVNNPJCJUPTFP-UHFFFAOYSA-N

**Formula:** C13H10ClF5O4

**SMILES:** O=C(CCC(=O)Oc1cccc(Cl)c1)OCC(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 360.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1286.78 | kJ/mol | Joback Method |
| hf | -1589.98 | kJ/mol | Joback Method |
| hfus | 33.42 | kJ/mol | Joback Method |
| hvap | 63.49 | kJ/mol | Joback Method |
| log10ws | -4.40 | | Crippen Method |
| logp | 3.766 | | Crippen Method |
| mcvol | 206.240 | ml/mol | McGowan Method |
| pc | 1920.30 | kPa | Joback Method |
| rinpol | 1678.00 | | NIST Webbook |
| rinpol | 1678.00 | | NIST Webbook |
| tb | 708.40 | K | Joback Method |
| tc | 901.23 | K | Joback Method |
| tf | 457.24 | K | Joback Method |
| vc | 0.821 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 558.24 | J/mol×K | 708.40 | Joback Method |
| cpg | 569.09 | J/mol×K | 740.54 | Joback Method |
| cpg | 579.11 | J/mol×K | 772.68 | Joback Method |
| cpg | 588.35 | J/mol×K | 804.81 | Joback Method |
| cpg | 596.86 | J/mol×K | 836.95 | Joback Method |
| cpg | 604.66 | J/mol×K | 869.09 | Joback Method |
| cpg | 611.81 | J/mol×K | 901.23 | Joback Method |

# Sources

| | |
|---|---|
| **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=U390871&Units=SI |

# 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 |