# Succinic acid, 2-chloro-6-fluorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

**Inchi:** InChI=1S/C14H10ClF7O4/c15-7-2-1-3-8(16)11(7)26-10(24)5-4-9(23)25-6-13(18,19)12(17

**InchiKey:** NAHHMBVLBJQYFA-UHFFFAOYSA-N

**Formula:** C14H10ClF7O4

**SMILES:** O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC(F)(F)C(F)C(F)(F)F

**Mol. weight [g/mol]:** 410.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1680.05 | kJ/mol | Joback Method |
| hf | -2019.59 | kJ/mol | Joback Method |
| hfus | 38.26 | kJ/mol | Joback Method |
| hvap | 64.36 | kJ/mol | Joback Method |
| log10ws | -5.12 | | Crippen Method |
| logp | 4.244 | | Crippen Method |
| mcvol | 223.870 | ml/mol | McGowan Method |
| pc | 1632.49 | kPa | Joback Method |
| rinpol | 1781.00 | | NIST Webbook |
| rinpol | 1781.00 | | NIST Webbook |
| tb | 734.36 | K | Joback Method |
| tc | 918.27 | K | Joback Method |
| tf | 467.21 | K | Joback Method |
| vc | 0.906 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 625.18 | J/mol×K | 734.36 | Joback Method |
| cpg | 635.71 | J/mol×K | 765.01 | Joback Method |
| cpg | 645.46 | J/mol×K | 795.66 | Joback Method |
| cpg | 654.48 | J/mol×K | 826.31 | Joback Method |
| cpg | 662.79 | J/mol×K | 856.96 | Joback Method |
| cpg | 670.43 | J/mol×K | 887.62 | Joback Method |
| cpg | 677.44 | J/mol×K | 918.27 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390807&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

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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 |