# Succinic acid, 2-chloro-6-fluorophenyl tetrahydrofurfuryl ester

**Inchi:** InChI=1S/C15H16ClFO5/c16-11-4-1-5-12(17)15(11)22-14(19)7-6-13(18)21-9-10-3-2-8-2(

**InchiKey:** XALIYFWWLKGVLV-UHFFFAOYSA-N

**Formula:** C15H16ClFO5

**SMILES:** O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC1CCCO1

**Mol. weight [g/mol]:** 330.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -555.58 | kJ/mol | Joback Method |
| hf | -912.31 | kJ/mol | Joback Method |
| hfus | 42.63 | kJ/mol | Joback Method |
| hvap | 79.23 | kJ/mol | Joback Method |
| log10ws | -3.69 | | Crippen Method |
| logp | 2.887 | | Crippen Method |
| mcvol | 222.350 | ml/mol | McGowan Method |
| pc | 2111.94 | kPa | Joback Method |
| rinpol | 2347.00 | | NIST Webbook |
| rinpol | 2347.00 | | NIST Webbook |
| tb | 810.75 | K | Joback Method |
| tc | 1031.30 | K | Joback Method |
| tf | 522.57 | K | Joback Method |
| vc | 0.845 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 645.95 | J/mol×K | 810.75 | Joback Method |
| cpg | 659.14 | J/mol×K | 847.51 | Joback Method |
| cpg | 671.18 | J/mol×K | 884.27 | Joback Method |
| cpg | 682.09 | J/mol×K | 921.02 | Joback Method |
| cpg | 691.89 | J/mol×K | 957.78 | Joback Method |
| cpg | 700.58 | J/mol×K | 994.54 | Joback Method |
| cpg | 708.20 | J/mol×K | 1031.30 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390721&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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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