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

**Inchi:** InChI=1S/C21H16ClFO4/c22-17-6-3-7-18(23)21(17)27-20(25)11-10-19(24)26-13-14-8-9-

**InchiKey:** FIKWBJBNJXAWSU-UHFFFAOYSA-N

**Formula:** C21H16ClFO4

**SMILES:** O=C(CCC(=O)Oc1c(F)cccc1Cl)OCc1ccc2ccccc2c1

**Mol. weight [g/mol]:** 386.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -246.06 | kJ/mol | Joback Method |
| hf | -548.50 | kJ/mol | Joback Method |
| hfus | 46.93 | kJ/mol | Joback Method |
| hvap | 92.40 | kJ/mol | Joback Method |
| log10ws | -6.83 | | Crippen Method |
| logp | 5.061 | | Crippen Method |
| mcvol | 268.660 | ml/mol | McGowan Method |
| pc | 1792.42 | kPa | Joback Method |
| rinpol | 3145.00 | | NIST Webbook |
| rinpol | 3145.00 | | NIST Webbook |
| tb | 956.44 | K | Joback Method |
| tc | 1194.46 | K | Joback Method |
| tf | 624.36 | K | Joback Method |
| vc | 1.032 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 784.34 | J/mol×K | 956.44 | Joback Method |
| cpg | 795.16 | J/mol×K | 996.11 | Joback Method |
| cpg | 804.89 | J/mol×K | 1035.78 | Joback Method |
| cpg | 813.60 | J/mol×K | 1075.45 | Joback Method |
| cpg | 821.35 | J/mol×K | 1115.12 | Joback Method |
| cpg | 828.21 | J/mol×K | 1154.79 | Joback Method |
| cpg | 834.26 | J/mol×K | 1194.46 | 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=U390006&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 |