# Succinic acid, 2-chloro-6-fluorophenyl 2-fluoro-3-(trifluoromethyl)phenyl ester

**Inchi:** InChI=1S/C17H10ClF5O4/c18-10-4-2-5-11(19)16(10)27-14(25)8-7-13(24)26-12-6-1-3-9(

**InchiKey:** XQEWRVKXKJTJDD-UHFFFAOYSA-N

**Formula:** C17H10ClF5O4

**SMILES:** O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1cccc(C(F)(F)F)c1F

**Mol. weight [g/mol]:** 408.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1172.42 | kJ/mol | Joback Method |
| hf | -1461.67 | kJ/mol | Joback Method |
| hfus | 44.07 | kJ/mol | Joback Method |
| hvap | 77.95 | kJ/mol | Joback Method |
| log10ws | -6.20 | | Crippen Method |
| logp | 4.928 | | Crippen Method |
| mcvol | 238.840 | ml/mol | McGowan Method |
| pc | 1737.56 | kPa | Joback Method |
| rinpol | 2256.00 | | NIST Webbook |
| rinpol | 2256.00 | | NIST Webbook |
| tb | 844.77 | K | Joback Method |
| tc | 1055.20 | K | Joback Method |
| tf | 563.88 | K | Joback Method |
| vc | 0.948 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 670.21 | J/mol×K | 844.77 | Joback Method |
| cpg | 680.16 | J/mol×K | 879.84 | Joback Method |
| cpg | 689.17 | J/mol×K | 914.91 | Joback Method |
| cpg | 697.26 | J/mol×K | 949.99 | Joback Method |
| cpg | 704.48 | J/mol×K | 985.06 | Joback Method |
| cpg | 710.85 | J/mol×K | 1020.13 | Joback Method |
| cpg | 716.40 | J/mol×K | 1055.20 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390787&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

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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 |