# Succinic acid, 4-fluorophenethyl 2-methylhex-3-yl ester

**Inchi:** InChI=1S/C19H27FO4/c1-4-5-17(14(2)3)24-19(22)11-10-18(21)23-13-12-15-6-8-16(20)9

**InchiKey:** YWSMKQGXZUYFIA-UHFFFAOYSA-N

**Formula:** C19H27FO4

**SMILES:** CCCC(OC(=O)CCC(=O)OCCc1ccc(F)cc1)C(C)C

**Mol. weight [g/mol]:** 338.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -455.65 | kJ/mol | Joback Method |
| hf | -906.70 | kJ/mol | Joback Method |
| hfus | 40.23 | kJ/mol | Joback Method |
| hvap | 77.55 | kJ/mol | Joback Method |
| log10ws | -4.81 | | Crippen Method |
| logp | 4.059 | | Crippen Method |
| mcvol | 271.460 | ml/mol | McGowan Method |
| pc | 1410.13 | kPa | Joback Method |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2200.00 | | NIST Webbook |
| tb | 816.75 | K | Joback Method |
| tc | 1015.50 | K | Joback Method |
| tf | 457.74 | K | Joback Method |
| vc | 1.046 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 827.58 | J/mol×K | 816.75 | Joback Method |
| cpg | 843.32 | J/mol×K | 849.87 | Joback Method |
| cpg | 857.97 | J/mol×K | 883.00 | Joback Method |
| cpg | 871.53 | J/mol×K | 916.12 | Joback Method |
| cpg | 884.03 | J/mol×K | 949.25 | Joback Method |
| cpg | 895.49 | J/mol×K | 982.37 | Joback Method |
| cpg | 905.94 | J/mol×K | 1015.50 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381299&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 |