# Succinic acid, 3-methylbut-2-yl pentafluorophenyl ester

**Inchi:** InChI=1S/C15H15F5O4/c1-6(2)7(3)23-8(21)4-5-9(22)24-15-13(19)11(17)10(16)12(18)14

**InchiKey:** VIOHWNFBZVGAPM-UHFFFAOYSA-N

**Formula:** C15H15F5O4

**SMILES:** CC(C)C(C)OC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 354.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1307.09 | kJ/mol | Joback Method |
| hf | -1654.46 | kJ/mol | Joback Method |
| hfus | 40.63 | kJ/mol | Joback Method |
| hvap | 68.02 | kJ/mol | Joback Method |
| log10ws | -5.11 | | Crippen Method |
| logp | 3.655 | | Crippen Method |
| mcvol | 222.180 | ml/mol | McGowan Method |
| pc | 1575.95 | kPa | Joback Method |
| rinpol | 1649.00 | | NIST Webbook |
| rinpol | 1649.00 | | NIST Webbook |
| tb | 742.23 | K | Joback Method |
| tc | 924.65 | K | Joback Method |
| tf | 465.10 | K | Joback Method |
| vc | 0.893 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 630.00 | J/mol×K | 742.23 | Joback Method |
| cpg | 642.30 | J/mol×K | 772.63 | Joback Method |
| cpg | 653.88 | J/mol×K | 803.04 | Joback Method |
| cpg | 664.72 | J/mol×K | 833.44 | Joback Method |
| cpg | 674.83 | J/mol×K | 863.84 | Joback Method |
| cpg | 684.20 | J/mol×K | 894.24 | Joback Method |
| cpg | 692.82 | J/mol×K | 924.65 | Joback Method |

# Sources

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|---|---|
| **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=U390347&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 |