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

**Inchi:** InChI=1S/C15H21F7O4/c1-4-5-10(9(2)3)26-12(24)7-6-11(23)25-8-13(16,17)14(18,19)15

**InchiKey:** IAWYKDRFTPIBSU-UHFFFAOYSA-N

**Formula:** C15H21F7O4

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

**Mol. weight [g/mol]:** 398.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1752.45 | kJ/mol | Joback Method |
| hf | -2252.11 | kJ/mol | Joback Method |
| hfus | 32.45 | kJ/mol | Joback Method |
| hvap | 56.91 | kJ/mol | Joback Method |
| log10ws | -4.99 | | Crippen Method |
| logp | 4.511 | | Crippen Method |
| mcvol | 249.480 | ml/mol | McGowan Method |
| pc | 1268.25 | kPa | Joback Method |
| rinpol | 1461.00 | | NIST Webbook |
| rinpol | 1461.00 | | NIST Webbook |
| tb | 679.50 | K | Joback Method |
| tc | 843.39 | K | Joback Method |
| tf | 384.52 | K | Joback Method |
| vc | 1.004 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 740.54 | J/mol×K | 679.50 | Joback Method |
| cpg | 754.75 | J/mol×K | 706.82 | Joback Method |
| cpg | 768.14 | J/mol×K | 734.13 | Joback Method |
| cpg | 780.75 | J/mol×K | 761.45 | Joback Method |
| cpg | 792.62 | J/mol×K | 788.76 | Joback Method |
| cpg | 803.78 | J/mol×K | 816.08 | Joback Method |
| cpg | 814.27 | J/mol×K | 843.39 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382352&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 |