# Succinic acid, 2,2,3,3-tetrafluoropropyl 3-nitrobenzyl ester

**Inchi:** InChI=1S/C14H13F4NO6/c15-13(16)14(17,18)8-25-12(21)5-4-11(20)24-7-9-2-1-3-10(6-9
**InchiKey:** FQTVEUWYOIOYMZ-UHFFFAOYSA-N
**Formula:** C14H13F4NO6
**SMILES:** O=C(CCC(=O)OCC(F)(F)C(F)F)OCc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 367.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1041.35 | kJ/mol | Joback Method |
| hf | -1406.06 | kJ/mol | Joback Method |
| hfus | 43.99 | kJ/mol | Joback Method |
| hvap | 79.65 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 2.862 | | Crippen Method |
| mcvol | 223.740 | ml/mol | McGowan Method |
| pc | 1898.60 | kPa | Joback Method |
| rinpol | 2219.00 | | NIST Webbook |
| rinpol | 2219.00 | | NIST Webbook |
| tb | 849.21 | K | Joback Method |
| tc | 1059.85 | K | Joback Method |
| tf | 564.19 | K | Joback Method |
| vc | 0.896 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 674.23 | J/mol×K | 849.21 | Joback Method |
| cpg | 684.45 | J/mol×K | 884.32 | Joback Method |
| cpg | 693.72 | J/mol×K | 919.42 | Joback Method |
| cpg | 702.07 | J/mol×K | 954.53 | Joback Method |
| cpg | 709.55 | J/mol×K | 989.64 | Joback Method |
| cpg | 716.19 | J/mol×K | 1024.74 | Joback Method |
| cpg | 722.03 | J/mol×K | 1059.85 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390176&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 |