# Succinic acid, 2,2-dichloroethyl 1,1,1-trifluoroprop-2-yl ester

**Inchi:** InChI=1S/C9H11Cl2F3O4/c1-5(9(12,13)14)18-8(16)3-2-7(15)17-4-6(10)11/h5-6H,2-4H2,

**InchiKey:** MPEONHWHNJQRGO-UHFFFAOYSA-N

**Formula:** C9H11Cl2F3O4

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

**Mol. weight [g/mol]:** 311.08

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1053.27 | kJ/mol | Joback Method |
| hf | -1357.81 | kJ/mol | Joback Method |
| hfus | 27.81 | kJ/mol | Joback Method |
| hvap | 58.19 | kJ/mol | Joback Method |
| log10ws | -3.00 | | Crippen Method |
| logp | 2.608 | | Crippen Method |
| mcvol | 182.340 | ml/mol | McGowan Method |
| pc | 2135.43 | kPa | Joback Method |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1421.00 | | NIST Webbook |
| tb | 626.46 | K | Joback Method |
| tc | 809.99 | K | Joback Method |
| tf | 369.54 | K | Joback Method |
| vc | 0.717 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 449.21 | J/mol×K | 626.46 | Joback Method |
| cpg | 459.77 | J/mol×K | 657.05 | Joback Method |
| cpg | 469.71 | J/mol×K | 687.64 | Joback Method |
| cpg | 479.05 | J/mol×K | 718.22 | Joback Method |
| cpg | 487.80 | J/mol×K | 748.81 | Joback Method |
| cpg | 495.98 | J/mol×K | 779.40 | Joback Method |
| cpg | 503.59 | J/mol×K | 809.99 | 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=U390842&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

| | |
|---|---|
| **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 |

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