

Succinic acid, 2,2,3,3-tetrafluoropropyl 2,2-dichloroethyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C9H10Cl2F4O4/c10-5(11)3-18-6(16)1-2-7(17)19-4-9(14,15)8(12)13/h5,8H,1-4H |
| InchiKey: | XUJITLGSPQOHOQ-UHFFFAOYSA-N |
| Formula: | C9H10Cl2F4O4 |
| SMILES: | O=C(CCC(=O)OCC(F)(F)C(F)F)OCC(Cl)Cl |
| Mol. weight [g/mol]: | 329.07 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -1248.08 | kJ/mol | Joback Method |
| hf | -1553.92 | kJ/mol | Joback Method |
| hfus | 30.89 | kJ/mol | Joback Method |
| hvap | 57.37 | kJ/mol | Joback Method |
| log10ws | -2.86 | | Crippen Method |
| logp | 2.557 | | Crippen Method |
| mcvol | 184.110 | ml/mol | McGowan Method |
| pc | 2049.31 | kPa | Joback Method |
| rinpol | 1532.00 | | NIST Webbook |
| rinpol | 1532.00 | | NIST Webbook |
| tb | 625.73 | K | Joback Method |
| tc | 802.44 | K | Joback Method |
| tf | 370.13 | K | Joback Method |
| vc | 0.735 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 457.36 | J/mol×K | 625.73 | Joback Method |
| cpg | 467.48 | J/mol×K | 655.18 | Joback Method |
| cpg | 477.03 | J/mol×K | 684.63 | Joback Method |
| cpg | 486.00 | J/mol×K | 714.08 | Joback Method |
| cpg | 494.42 | J/mol×K | 743.53 | Joback Method |
| cpg | 502.29 | J/mol×K | 772.98 | Joback Method |
| cpg | 509.64 | J/mol×K | 802.44 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390514&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.cheméo.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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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