# Succinic acid, propyl 2,2,2-trichloroethyl ester

**Inchi:** InChI=1S/C9H13Cl3O4/c1-2-5-15-7(13)3-4-8(14)16-6-9(10,11)12/h2-6H2,1H3
**InchiKey:** XDAKQGGVMSYSGN-UHFFFAOYSA-N
**Formula:** C9H13Cl3O4
**SMILES:** CCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 291.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -475.89 | kJ/mol | Joback Method |
| hf | -774.66 | kJ/mol | Joback Method |
| hfus | 29.82 | kJ/mol | Joback Method |
| hvap | 65.80 | kJ/mol | Joback Method |
| log10ws | -2.88 | | Crippen Method |
| logp | 2.633 | | Crippen Method |
| mcvol | 189.270 | ml/mol | McGowan Method |
| pc | 2306.95 | kPa | Joback Method |
| rinpol | 1656.00 | | NIST Webbook |
| tb | 666.96 | K | Joback Method |
| tc | 871.06 | K | Joback Method |
| tf | 427.69 | K | Joback Method |
| vc | 0.724 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 447.73 | J/mol×K | 666.96 | Joback Method |
| cpg | 458.47 | J/mol×K | 700.98 | Joback Method |
| cpg | 468.53 | J/mol×K | 734.99 | Joback Method |
| cpg | 477.90 | J/mol×K | 769.01 | Joback Method |
| cpg | 486.62 | J/mol×K | 803.03 | Joback Method |
| cpg | 494.70 | J/mol×K | 837.05 | Joback Method |
| cpg | 502.14 | J/mol×K | 871.06 | Joback Method |
| dvisc | 0.0012886 | Pa×s | 427.69 | Joback Method |
| dvisc | 0.0007598 | Pa×s | 467.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004868 | Pa×s | 507.45 | Joback Method |
| dvisc | 0.0003328 | Pa×s | 547.33 | Joback Method |
| dvisc | 0.0002396 | Pa×s | 587.20 | Joback Method |
| dvisc | 0.0001798 | Pa×s | 627.08 | Joback Method |
| dvisc | 0.0001397 | Pa×s | 666.96 | Joback Method |

# Sources

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|---|---|
| **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=U349165&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |