# Succinic acid, 2-(adamant-1-yl)ethyl 2,2-dichloroethyl ester

**Inchi:** InChI=1S/C18H26Cl2O4/c19-15(20)11-24-17(22)2-1-16(21)23-4-3-18-8-12-5-13(9-18)7-1

**InchiKey:** UQWXAYDLHHYETA-UHFFFAOYSA-N

**Formula:** C18H26Cl2O4

**SMILES:** O=C(CCC(=O)OCC(Cl)Cl)OCCC12CC3CC(CC(C3)C1)C2

**Mol. weight [g/mol]:** 377.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -236.51 | kJ/mol | Joback Method |
| hf | -734.07 | kJ/mol | Joback Method |
| hfus | 39.90 | kJ/mol | Joback Method |
| hvap | 80.81 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 4.263 | | Crippen Method |
| mcvol | 271.260 | ml/mol | McGowan Method |
| pc | 1609.00 | kPa | Joback Method |
| rinpol | 2770.00 | | NIST Webbook |
| rinpol | 2770.00 | | NIST Webbook |
| tb | 858.30 | K | Joback Method |
| tc | 1076.71 | K | Joback Method |
| tf | 551.74 | K | Joback Method |
| vc | 1.044 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 865.27 | J/mol×K | 858.30 | Joback Method |
| cpg | 883.57 | J/mol×K | 894.70 | Joback Method |
| cpg | 901.49 | J/mol×K | 931.10 | Joback Method |
| cpg | 919.23 | J/mol×K | 967.51 | Joback Method |
| cpg | 936.97 | J/mol×K | 1003.91 | Joback Method |
| cpg | 954.89 | J/mol×K | 1040.31 | Joback Method |
| cpg | 973.18 | J/mol×K | 1076.71 | 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=U391365&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |