# Succinic acid, propyl 2,3,5-trichlorophenyl ester

**Inchi:** InChI=1S/C13H13Cl3O4/c1-2-5-19-11(17)3-4-12(18)20-10-7-8(14)6-9(15)13(10)16/h6-7H

**InchiKey:** BCWDFFKPKYQWFC-UHFFFAOYSA-N

**Formula:** C13H13Cl3O4

**SMILES:** CCCOC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1Cl

**Mol. weight [g/mol]:** 339.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -361.53 | kJ/mol | Joback Method |
| hf | -646.35 | kJ/mol | Joback Method |
| hfus | 40.46 | kJ/mol | Joback Method |
| hvap | 80.26 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.286 | | Crippen Method |
| mcvol | 221.870 | ml/mol | McGowan Method |
| pc | 2068.00 | kPa | Joback Method |
| rinpol | 2209.00 | | NIST Webbook |
| tb | 803.33 | K | Joback Method |
| tc | 1023.24 | K | Joback Method |
| tf | 534.33 | K | Joback Method |
| vc | 0.851 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 555.95 | J/mol×K | 803.33 | Joback Method |
| cpg | 599.88 | J/mol×K | 986.59 | Joback Method |
| cpg | 592.88 | J/mol×K | 949.93 | Joback Method |
| cpg | 584.99 | J/mol×K | 913.28 | Joback Method |
| cpg | 576.20 | J/mol×K | 876.63 | Joback Method |
| cpg | 566.52 | J/mol×K | 839.98 | Joback Method |
| cpg | 605.98 | J/mol×K | 1023.24 | Joback Method |
| dvisc | 0.0000969 | Pa×s | 803.33 | Joback Method |
| dvisc | 0.0001178 | Pa×s | 758.50 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001469 | Pa×s | 713.66 | Joback Method |
| dvisc | 0.0001887 | Pa×s | 668.83 | Joback Method |
| dvisc | 0.0002513 | Pa×s | 624.00 | Joback Method |
| dvisc | 0.0003497 | Pa×s | 579.16 | Joback Method |
| dvisc | 0.0005145 | Pa×s | 534.33 | 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=U349606&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 |
| **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 |