# Propanoic acid, 2,2,2-trichloroethyl ester

**Other names:** 2,2,2-Trichloroethyl propionate
2,2,2-Trichloroethyl propanoate
**Inchi:** InChI=1S/C5H7Cl3O2/c1-2-4(9)10-3-5(6,7)8/h2-3H2,1H3
**InchiKey:** MEFWWUOADZDECZ-UHFFFAOYSA-N
**Formula:** C5H7Cl3O2
**SMILES:** CCC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 205.47

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -275.65 | kJ/mol | Joback Method |
| hf | -447.30 | kJ/mol | Joback Method |
| hfus | 16.67 | kJ/mol | Joback Method |
| hvap | 47.74 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Crippen Method |
| logp | 2.310 | | Crippen Method |
| mcvol | 125.470 | ml/mol | McGowan Method |
| pc | 3287.81 | kPa | Joback Method |
| rinpol | 1080.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1101.00 | | NIST Webbook |
| rinpol | 1094.00 | | NIST Webbook |
| rinpol | 1089.00 | | NIST Webbook |
| rinpol | 1087.00 | | NIST Webbook |
| rinpol | 1057.00 | | NIST Webbook |
| ripol | 1503.00 | | NIST Webbook |
| ripol | 1484.00 | | NIST Webbook |
| ripol | 1484.00 | | NIST Webbook |
| ripol | 1504.00 | | NIST Webbook |
| ripol | 1494.00 | | NIST Webbook |
| ripol | 1532.00 | | NIST Webbook |
| tb | 499.15 | K | Joback Method |
| tc | 710.20 | K | Joback Method |
| tf | 310.45 | K | Joback Method |
| vc | 0.475 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 234.65 | J/mol×K | 499.15 | Joback Method |
| cpg | 271.22 | J/mol×K | 675.02 | Joback Method |
| cpg | 264.90 | J/mol×K | 639.85 | Joback Method |
| cpg | 258.10 | J/mol×K | 604.67 | Joback Method |
| cpg | 250.81 | J/mol×K | 569.50 | Joback Method |
| cpg | 243.00 | J/mol×K | 534.32 | Joback Method |
| cpg | 277.09 | J/mol×K | 710.20 | Joback Method |
| dvisc | 0.0003190 | Pa×s | 499.15 | Joback Method |
| dvisc | 0.0004123 | Pa×s | 467.70 | Joback Method |
| dvisc | 0.0005530 | Pa×s | 436.25 | Joback Method |
| dvisc | 0.0007762 | Pa×s | 404.80 | Joback Method |
| dvisc | 0.0011536 | Pa×s | 373.35 | Joback Method |
| dvisc | 0.0018441 | Pa×s | 341.90 | Joback Method |
| dvisc | 0.0032418 | Pa×s | 310.45 | 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=R19783&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 |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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