# 2,2,2-Trichloroethyl undecanoate

**Inchi:** InChI=1S/C13H23Cl3O2/c1-2-3-4-5-6-7-8-9-10-12(17)18-11-13(14,15)16/h2-11H2,1H3
**InchiKey:** ZBXABUUOULPNKG-UHFFFAOYSA-N
**Formula:** C13H23Cl3O2
**SMILES:** CCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 317.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -208.29 | kJ/mol | Joback Method |
| hf | -612.42 | kJ/mol | Joback Method |
| hfus | 37.39 | kJ/mol | Joback Method |
| hvap | 65.55 | kJ/mol | Joback Method |
| log10ws | -5.69 | | Crippen Method |
| logp | 5.431 | | Crippen Method |
| mcvol | 238.190 | ml/mol | McGowan Method |
| pc | 1584.75 | kPa | Joback Method |
| rinpol | 1875.00 | | NIST Webbook |
| rinpol | 1877.00 | | NIST Webbook |
| rinpol | 1877.00 | | NIST Webbook |
| rinpol | 1876.00 | | NIST Webbook |
| rinpol | 1875.00 | | NIST Webbook |
| rinpol | 1875.00 | | NIST Webbook |
| ripol | 2264.00 | | NIST Webbook |
| ripol | 2240.00 | | NIST Webbook |
| ripol | 2244.00 | | NIST Webbook |
| ripol | 2281.00 | | NIST Webbook |
| ripol | 2224.00 | | NIST Webbook |
| ripol | 2237.00 | | NIST Webbook |
| ripol | 2260.00 | | NIST Webbook |
| tb | 682.19 | K | Joback Method |
| tc | 872.30 | K | Joback Method |
| tf | 400.61 | K | Joback Method |
| vc | 0.923 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 611.33 | J/mol×K | 682.19 | Joback Method |
| cpg | 625.80 | J/mol×K | 713.87 | Joback Method |
| cpg | 639.46 | J/mol×K | 745.56 | Joback Method |
| cpg | 652.33 | J/mol×K | 777.24 | Joback Method |
| cpg | 664.47 | J/mol×K | 808.93 | Joback Method |
| cpg | 675.89 | J/mol×K | 840.61 | Joback Method |
| cpg | 686.64 | J/mol×K | 872.30 | Joback Method |
| dvisc | 0.0016819 | Pa×s | 400.61 | Joback Method |
| dvisc | 0.0008389 | Pa×s | 447.54 | Joback Method |
| dvisc | 0.0004775 | Pa×s | 494.47 | Joback Method |
| dvisc | 0.0002997 | Pa×s | 541.40 | Joback Method |
| dvisc | 0.0002026 | Pa×s | 588.33 | Joback Method |
| dvisc | 0.0001451 | Pa×s | 635.26 | Joback Method |
| dvisc | 0.0001088 | Pa×s | 682.19 | Joback Method |

# Sources

**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=R30559&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# 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

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|---|---|
| **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 |