# 2,2,2-Trichloroethyl hexadecanoate

**Inchi:** InChI=1S/C18H33Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17(22)23-16-18(19,20)21
**InchiKey:** FDHHGSHXWKVBKR-UHFFFAOYSA-N
**Formula:** C18H33Cl3O2
**SMILES:** CCCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 387.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -166.19 | kJ/mol | Joback Method |
| hf | -715.62 | kJ/mol | Joback Method |
| hfus | 50.34 | kJ/mol | Joback Method |
| hvap | 76.68 | kJ/mol | Joback Method |
| log10ws | -7.78 | | Crippen Method |
| logp | 7.381 | | Crippen Method |
| mcvol | 308.640 | ml/mol | McGowan Method |
| pc | 1117.06 | kPa | Joback Method |
| rinpol | 2378.00 | | NIST Webbook |
| rinpol | 2376.00 | | NIST Webbook |
| rinpol | 2377.00 | | NIST Webbook |
| rinpol | 2377.00 | | NIST Webbook |
| ripol | 2767.00 | | NIST Webbook |
| ripol | 2747.00 | | NIST Webbook |
| ripol | 2747.00 | | NIST Webbook |
| ripol | 2766.00 | | NIST Webbook |
| ripol | 2772.00 | | NIST Webbook |
| ripol | 2783.00 | | NIST Webbook |
| ripol | 2767.00 | | NIST Webbook |
| tb | 796.59 | K | Joback Method |
| tc | 985.44 | K | Joback Method |
| tf | 456.96 | K | Joback Method |
| vc | 1.204 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 891.14 | J/mol×K | 796.59 | Joback Method |
| cpg | 964.18 | J/mol×K | 953.96 | Joback Method |
| cpg | 951.25 | J/mol×K | 922.49 | Joback Method |
| cpg | 937.52 | J/mol×K | 891.01 | Joback Method |
| cpg | 922.96 | J/mol×K | 859.54 | Joback Method |
| cpg | 907.51 | J/mol×K | 828.06 | Joback Method |
| cpg | 976.37 | J/mol×K | 985.44 | Joback Method |
| dvisc | 0.0000507 | Pa×s | 796.59 | Joback Method |
| dvisc | 0.0000685 | Pa×s | 739.99 | Joback Method |
| dvisc | 0.0000972 | Pa×s | 683.38 | Joback Method |
| dvisc | 0.0001469 | Pa×s | 626.77 | Joback Method |
| dvisc | 0.0002411 | Pa×s | 570.17 | Joback Method |
| dvisc | 0.0004414 | Pa×s | 513.56 | Joback Method |
| dvisc | 0.0009387 | Pa×s | 456.96 | Joback Method |

# Sources

**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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R30456&Units=SI

# 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 |