# 2,2,2-Trichloroethyl octanoate

**Other names:** Octanoic acid, 2,2,2-trichloroethyl ester
**Inchi:** InChI=1S/C10H17Cl3O2/c1-2-3-4-5-6-7-9(14)15-8-10(11,12)13/h2-8H2,1H3
**InchiKey:** HSGDHOUWEKLJIE-UHFFFAOYSA-N
**Formula:** C10H17Cl3O2
**SMILES:** CCCCCCCC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 275.60

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -233.55 | kJ/mol | Joback Method |
| hf | -550.50 | kJ/mol | Joback Method |
| hfus | 29.62 | kJ/mol | Joback Method |
| hvap | 58.87 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 4.260 | | Crippen Method |
| mcvol | 195.920 | ml/mol | McGowan Method |
| pc | 2021.76 | kPa | Joback Method |
| rinpol | 1579.00 | | NIST Webbook |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1577.00 | | NIST Webbook |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1574.00 | | NIST Webbook |
| rinpol | 1577.00 | | NIST Webbook |
| rinpol | 1561.00 | | NIST Webbook |
| rinpol | 1579.00 | | NIST Webbook |
| rinpol | 1561.00 | | NIST Webbook |
| ripol | 1938.00 | | NIST Webbook |
| ripol | 1966.00 | | NIST Webbook |
| ripol | 1956.00 | | NIST Webbook |
| ripol | 1997.00 | | NIST Webbook |
| ripol | 1928.00 | | NIST Webbook |
| ripol | 1948.00 | | NIST Webbook |
| ripol | 1940.00 | | NIST Webbook |
| ripol | 1940.00 | | NIST Webbook |
| tb | 613.55 | K | Joback Method |
| tc | 809.74 | K | Joback Method |

| | | | |
|---|---|---|---|
| tf | 366.80 | K | Joback Method |
| vc | 0.755 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 458.10 | J/mol×K | 613.55 | Joback Method |
| cpg | 515.31 | J/mol×K | 777.04 | Joback Method |
| cpg | 505.23 | J/mol×K | 744.35 | Joback Method |
| cpg | 494.50 | J/mol×K | 711.65 | Joback Method |
| cpg | 483.09 | J/mol×K | 678.95 | Joback Method |
| cpg | 470.97 | J/mol×K | 646.25 | Joback Method |
| cpg | 524.77 | J/mol×K | 809.74 | Joback Method |
| dvisc | 0.0001674 | Pa×s | 613.55 | Joback Method |
| dvisc | 0.0002210 | Pa×s | 572.42 | Joback Method |
| dvisc | 0.0003047 | Pa×s | 531.30 | Joback Method |
| dvisc | 0.0004433 | Pa×s | 490.17 | Joback Method |
| dvisc | 0.0006909 | Pa×s | 449.05 | Joback Method |
| dvisc | 0.0011775 | Pa×s | 407.93 | Joback Method |
| dvisc | 0.0022618 | Pa×s | 366.80 | 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=R19961&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 |
| **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 |

Latest version available from:

https://www.chemeo.com/cid/10-943-3/2-2-2-Trichloroethyl-octanoate.pdf

Generated by Cheméo on 2024-10-12 08:59:38.971033093 +0000 UTC m=+3304441.608002342.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.