# 1,14-Dichloro-3,6,12-trithia-9-oxatetradecane

**Inchi:** InChI=1S/C10H20Cl2OS3/c11-1-5-14-7-3-13-4-8-16-10-9-15-6-2-12/h1-10H2
**InchiKey:** CSWFFQYKMQIBDP-UHFFFAOYSA-N
**Formula:** C10H20Cl2OS3
**SMILES:** ClCCSCCOCCSCCSCCCl
**Mol. weight [g/mol]:** 323.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 3.82 | kJ/mol | Joback Method |
| hf | -287.82 | kJ/mol | Joback Method |
| hfus | 43.63 | kJ/mol | Joback Method |
| hvap | 69.48 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 3.680 | | Crippen Method |
| mcvol | 231.160 | ml/mol | McGowan Method |
| pc | 2032.72 | kPa | Joback Method |
| rinpol | 2419.00 | | NIST Webbook |
| rinpol | 2514.50 | | NIST Webbook |
| rinpol | 2419.00 | | NIST Webbook |
| rinpol | 2419.00 | | NIST Webbook |
| rinpol | 2514.50 | | NIST Webbook |
| tb | 731.82 | K | Joback Method |
| tc | 952.39 | K | Joback Method |
| tf | 387.73 | K | Joback Method |
| vc | 0.874 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 572.24 | J/mol×K | 731.82 | Joback Method |
| cpg | 585.96 | J/mol×K | 768.58 | Joback Method |
| cpg | 598.71 | J/mol×K | 805.34 | Joback Method |
| cpg | 610.50 | J/mol×K | 842.10 | Joback Method |
| cpg | 621.32 | J/mol×K | 878.86 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 631.16 | J/mol×K | 915.63 | Joback Method |
| cpg | 640.03 | J/mol×K | 952.39 | 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=R41392&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |