# Triethylene glycol, thio, S-octyl

**Inchi:** InChI=1S/C14H30O3S/c1-2-3-4-5-6-7-13-18-14-12-17-11-10-16-9-8-15/h15H,2-14H2,1H
**InchiKey:** PQTOSHDDJMDWTF-UHFFFAOYSA-N
**Formula:** C14H30O3S
**SMILES:** CCCCCCCCSCCOCCOCCO
**Mol. weight [g/mol]:** 278.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -246.70 | kJ/mol | Joback Method |
| hf | -707.09 | kJ/mol | Joback Method |
| hfus | 42.61 | kJ/mol | Joback Method |
| hvap | 75.07 | kJ/mol | Joback Method |
| log10ws | -3.00 | | Crippen Method |
| logp | 3.106 | | Crippen Method |
| mcvol | 242.080 | ml/mol | McGowan Method |
| pc | 1616.77 | kPa | Joback Method |
| rinpol | 2123.00 | | NIST Webbook |
| rinpol | 2123.00 | | NIST Webbook |
| tb | 725.52 | K | Joback Method |
| tc | 899.95 | K | Joback Method |
| tf | 387.22 | K | Joback Method |
| vc | 0.928 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 707.00 | J/mol×K | 725.52 | Joback Method |
| cpg | 722.50 | J/mol×K | 754.59 | Joback Method |
| cpg | 737.24 | J/mol×K | 783.66 | Joback Method |
| cpg | 751.24 | J/mol×K | 812.74 | Joback Method |
| cpg | 764.50 | J/mol×K | 841.81 | Joback Method |
| cpg | 777.02 | J/mol×K | 870.88 | Joback Method |
| cpg | 788.81 | J/mol×K | 899.95 | Joback Method |

# Sources

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|---|---|
| **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=R120086&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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