

trans-2,5-Dimethyl-1,3-oxathiolane

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| Inchi: | InChI=1S/C5H10OS/c1-4-3-7-5(2)6-4/h4-5H,3H2,1-2H3/t4-,5+/m0/s1 |
| InchiKey: | HLLCFXLPRUGRGF-CRCLSJGQSA-N |
| Formula: | C5H10OS |
| SMILES: | CC1CSC(C)O1 |
| Mol. weight [g/mol]: | 118.20 |
| CAS: | 38348-51-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -26.20 | kJ/mol | Joback Method |
| hf | -193.13 | kJ/mol | Joback Method |
| hfus | 15.35 | kJ/mol | Joback Method |
| hvap | 36.99 | kJ/mol | Joback Method |
| log10ws | -1.50 | | Crippen Method |
| logp | 1.484 | | Crippen Method |
| mcvol | 92.670 | ml/mol | McGowan Method |
| pc | 4077.71 | kPa | Joback Method |
| tb | 399.19 | K | Joback Method |
| tc | 613.97 | K | Joback Method |
| tf | 262.79 | K | Joback Method |
| vc | 0.323 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 172.65 | J/molxK | 399.19 | Joback Method |
| cpg | 185.37 | J/molxK | 434.99 | Joback Method |
| cpg | 197.47 | J/molxK | 470.78 | Joback Method |
| cpg | 208.94 | J/molxK | 506.58 | Joback Method |
| cpg | 219.82 | J/molxK | 542.38 | Joback Method |
| cpg | 230.11 | J/molxK | 578.17 | Joback Method |
| cpg | 239.83 | J/molxK | 613.97 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38348515&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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