

1,4-Oxathiane, 4,4-dioxide

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| Other names: | 1,4-Oxathiane sulfone 1,4-Thioxane-1,1-dioxide 1,4-oxathiane 4,4-dioxide Oxathiane 4,4-dioxide Thioxane sulfone USAF do-38 p-Oxathiane-4,4-dioxide p-Thioxane sulfone |
| Inchi: | InChI=1S/C4H8O3S/c5-8(6)3-1-7-2-4-8/h1-4H2 |
| InchiKey: | WWRUZECKUVNAPB-UHFFFAOYSA-N |
| Formula: | C4H8O3S |
| SMILES: | O=S1(=O)CCOCC1 |
| Mol. weight [g/mol]: | 136.17 |
| CAS: | 107-61-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------------|----------------------|--|
| gf | -532.96 | kJ/mol | Joback Method |
| hf | -633.19 | kJ/mol | Joback Method |
| hfus | 20.20 | kJ/mol | Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives |
| hsub | 92.00 ± 1.00 | kJ/mol | NIST Webbook |
| hvap | 47.38 | kJ/mol | Joback Method |
| log10ws | 0.69 | | Crippen Method |
| logp | -0.569 | | Crippen Method |
| mcvol | 90.320 | ml/mol | McGowan Method |
| pc | 6493.16 | kPa | Joback Method |
| tb | 368.92 | K | Joback Method |
| tc | 563.20 | K | Joback Method |
| tf | 260.64 | K | Joback Method |
| vc | 0.333 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------------|---------|-----------------|---------------|
| cpg | 155.38 | J/mol×K | 368.92 | Joback Method |
| cpg | 167.09 | J/mol×K | 401.30 | Joback Method |
| cpg | 178.26 | J/mol×K | 433.68 | Joback Method |
| cpg | 188.88 | J/mol×K | 466.06 | Joback Method |
| cpg | 198.96 | J/mol×K | 498.44 | Joback Method |
| cpg | 208.52 | J/mol×K | 530.82 | Joback Method |
| cpg | 217.55 | J/mol×K | 563.20 | Joback Method |
| hsubt | 91.60 ± 1.00 | kJ/mol | 314.50 | NIST Webbook |

Sources

| | |
|---|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C107619&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives: | https://www.doi.org/10.1016/j.tca.2005.11.024 |
| 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 |
| hsub: | Enthalpy of sublimation at standard conditions |
| hsubt: | Enthalpy of sublimation at a given temperature |
| hvp: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mvol: | 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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