# m-Dithiane, 1-oxide

**Other names:** 1,3-Dithiane, 1-oxide
1,3-Dithiane sulfoxide
**Inchi:** InChI=1S/C4H8OS2/c5-7-3-1-2-6-4-7/h1-4H2
**InchiKey:** ONTCBWKSXDATLL-UHFFFAOYSA-N
**Formula:** C4H8OS2
**SMILES:** O=S1CCCSC1
**Mol. weight [g/mol]:** 136.24
**CAS:** 16487-10-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -156.15 | kJ/mol | Joback Method |
| hf | -208.32 | kJ/mol | Joback Method |
| hfus | 7.82 | kJ/mol | Joback Method |
| hvap | 42.77 | kJ/mol | Joback Method |
| log10ws | -0.41 | | Crippen Method |
| logp | 0.830 | | Crippen Method |
| mcvol | 94.930 | ml/mol | McGowan Method |
| pc | 5853.95 | kPa | Joback Method |
| tb | 400.30 | K | Joback Method |
| tc | 628.72 | K | Joback Method |
| tf | 315.44 | K | Joback Method |
| vc | 0.322 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 158.55 | J/mol×K | 400.30 | Joback Method |
| cpg | 170.82 | J/mol×K | 438.37 | Joback Method |
| cpg | 182.34 | J/mol×K | 476.44 | Joback Method |
| cpg | 193.14 | J/mol×K | 514.51 | Joback Method |
| cpg | 203.24 | J/mol×K | 552.58 | Joback Method |
| cpg | 212.67 | J/mol×K | 590.65 | Joback Method |
| cpg | 221.45 | J/mol×K | 628.72 | Joback Method |

| | | | | |
|---|---|---|---|---|
| hfust | 22.60 | kJ/mol | 361.90 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C16487108&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |