# 4-Methyl-1,2,3-trithiolane

**Inchi:** InChI=1S/C3H6S3/c1-3-2-4-6-5-3/h3H,2H2,1H3
**InchiKey:** MBYUXUPOTRBMDQ-UHFFFAOYSA-N
**Formula:** C3H6S3
**SMILES:** CC1CSSS1
**Mol. weight [g/mol]:** 138.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 52.82 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 8.43 | kJ/mol | Joback Method |
| ie | 8.42 | eV | Cheméo Relay (1.0) |
| logp | 2.418 | | Crippen Method |
| mcvol | 91.320 | ml/mol | McGowan Method |
| rinpol | 1157.30 | | NIST Webbook |
| tb | 494.61 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 151.28 | J/mol×K | 426.81 | Joback Method |
| cpg | 161.14 | J/mol×K | 469.90 | Joback Method |
| cpg | 170.27 | J/mol×K | 512.99 | Joback Method |
| cpg | 178.72 | J/mol×K | 556.08 | Joback Method |
| cpg | 186.53 | J/mol×K | 599.17 | Joback Method |
| cpg | 193.74 | J/mol×K | 642.26 | Joback Method |
| cpg | 200.40 | J/mol×K | 685.35 | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C116664290&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |