# 1,2,5-trithiacyclooctane

**Inchi:** InChI=1S/C5H10S3/c1-2-6-4-5-8-7-3-1/h1-5H2
**InchiKey:** NYYXNYALXKWFOR-UHFFFAOYSA-N
**Formula:** C5H10S3
**SMILES:** C1CSCCSSC1
**Mol. weight [g/mol]:** 166.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 118.76 | kJ/mol | Joback Method |
| hf | 51.59 | kJ/mol | Joback Method |
| hfus | 6.24 | kJ/mol | Joback Method |
| hvap | 45.24 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.505 | | Crippen Method |
| mcvol | 119.500 | ml/mol | McGowan Method |
| pc | 4903.92 | kPa | Joback Method |
| rinpol | 1297.00 | | NIST Webbook |
| rinpol | 1302.00 | | NIST Webbook |
| rinpol | 1302.00 | | NIST Webbook |
| tb | 490.05 | K | Joback Method |
| tc | 772.16 | K | Joback Method |
| tf | 401.04 | K | Joback Method |
| vc | 0.371 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 223.91 | J/mol×K | 490.05 | Joback Method |
| cpg | 239.70 | J/mol×K | 537.07 | Joback Method |
| cpg | 254.32 | J/mol×K | 584.09 | Joback Method |
| cpg | 267.82 | J/mol×K | 631.11 | Joback Method |
| cpg | 280.22 | J/mol×K | 678.12 | Joback Method |
| cpg | 291.56 | J/mol×K | 725.14 | Joback Method |
| cpg | 301.86 | J/mol×K | 772.16 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R222518&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |