# 3-methyl-4-thianonane

**Inchi:** InChI=1S/C9H20S/c1-4-6-7-8-10-9(3)5-2/h9H,4-8H2,1-3H3
**InchiKey:** VKQVRBILRUNEDJ-UHFFFAOYSA-N
**Formula:** C9H20S
**SMILES:** CCCCCSC(C)CC
**Mol. weight [g/mol]:** 160.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 55.58 | kJ/mol | Joback Method |
| hf | -192.50 | kJ/mol | Joback Method |
| hfus | 19.67 | kJ/mol | Joback Method |
| hvap | 42.06 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.708 | | Crippen Method |
| mcvol | 154.020 | ml/mol | McGowan Method |
| pc | 2363.37 | kPa | Joback Method |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| tb | 473.66 | K | Joback Method |
| tc | 661.48 | K | Joback Method |
| tf | 210.59 | K | Joback Method |
| vc | 0.588 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 330.57 | J/mol×K | 473.66 | Joback Method |
| cpg | 345.86 | J/mol×K | 504.96 | Joback Method |
| cpg | 360.50 | J/mol×K | 536.27 | Joback Method |
| cpg | 374.52 | J/mol×K | 567.57 | Joback Method |
| cpg | 387.92 | J/mol×K | 598.87 | Joback Method |
| cpg | 400.72 | J/mol×K | 630.17 | Joback Method |
| cpg | 412.93 | J/mol×K | 661.48 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R156753&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 |

# 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 |