# Pentacosane, 1,2-bis(methylthio)

**Inchi:** InChI=1S/C27H56S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-
**InchiKey:** HZAHQJWPGNXPCN-UHFFFAOYSA-N
**Formula:** C27H56S2
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC
**Mol. weight [g/mol]:** 444.86

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 240.26 | kJ/mol | Joback Method |
| hf | -522.15 | kJ/mol | Joback Method |
| hfus | 70.42 | kJ/mol | Joback Method |
| hvap | 88.94 | kJ/mol | Joback Method |
| log10ws | -11.00 | | Crippen Method |
| logp | 10.683 | | Crippen Method |
| mcvol | 423.990 | ml/mol | McGowan Method |
| pc | 704.33 | kPa | Joback Method |
| rinpol | 3324.00 | | NIST Webbook |
| rinpol | 3324.00 | | NIST Webbook |
| tb | 954.28 | K | Joback Method |
| tc | 1170.03 | K | Joback Method |
| tf | 447.85 | K | Joback Method |
| vc | 1.649 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1437.69 | J/mol×K | 954.28 | Joback Method |
| cpg | 1460.17 | J/mol×K | 990.24 | Joback Method |
| cpg | 1481.08 | J/mol×K | 1026.20 | Joback Method |
| cpg | 1500.47 | J/mol×K | 1062.16 | Joback Method |
| cpg | 1518.42 | J/mol×K | 1098.11 | Joback Method |
| cpg | 1535.00 | J/mol×K | 1134.07 | Joback Method |
| cpg | 1550.29 | J/mol×K | 1170.03 | Joback Method |

# Sources

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|---|---|
| **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=R59321&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 |
| **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 |