

bis(3-methylbut-3-enyl) disulfide

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| Inchi: | InChI=1S/C10H18S2/c1-9(2)5-7-11-12-8-6-10(3)4/h1,3,5-8H2,2,4H3 |
| InchiKey: | PJAJDNBIZBZBGO-UHFFFAOYSA-N |
| Formula: | C10H18S2 |
| SMILES: | C=C(C)CCSSCCC(=C)C |
| Mol. weight [g/mol]: | 202.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 258.14 | kJ/mol | Joback Method |
| hf | 65.29 | kJ/mol | Joback Method |
| hfus | 24.74 | kJ/mol | Joback Method |
| hvap | 50.31 | kJ/mol | Joback Method |
| log10ws | -4.47 | | Crippen Method |
| logp | 4.300 | | Crippen Method |
| mcvol | 175.860 | ml/mol | McGowan Method |
| pc | 2379.54 | kPa | Joback Method |
| rinpol | 1437.00 | | NIST Webbook |
| rinpol | 1437.00 | | NIST Webbook |
| rinpol | 1441.00 | | NIST Webbook |
| tb | 558.88 | K | Joback Method |
| tc | 774.73 | K | Joback Method |
| tf | 239.82 | K | Joback Method |
| vc | 0.667 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 394.75 | J/mol×K | 558.88 | Joback Method |
| cpg | 410.14 | J/mol×K | 594.85 | Joback Method |
| cpg | 424.68 | J/mol×K | 630.83 | Joback Method |
| cpg | 438.39 | J/mol×K | 666.80 | Joback Method |
| cpg | 451.31 | J/mol×K | 702.78 | Joback Method |
| cpg | 463.46 | J/mol×K | 738.75 | Joback Method |
| cpg | 474.86 | J/mol×K | 774.73 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R493002&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

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 |
| rlnpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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