

(E) 1,2-Di(ethylthio)ethene

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H12S2/c1-3-7-5-6-8-4-2/h5-6H,3-4H2,1-2H3/b6-5+ |
| InchiKey: | DLMKAVFNJZJSNR-AATRIKPKSA-N |
| Formula: | C6H12S2 |
| SMILES: | CCSC=CSCC |
| Mol. weight [g/mol]: | 148.29 |
| CAS: | 14044-68-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 146.10 | kJ/mol | Joback Method |
| hf | 33.79 | kJ/mol | Joback Method |
| hfus | 19.76 | kJ/mol | Joback Method |
| hvap | 42.54 | kJ/mol | Joback Method |
| log10ws | -2.95 | | Crippen Method |
| logp | 2.964 | | Crippen Method |
| mcvol | 123.800 | ml/mol | McGowan Method |
| pc | 3427.87 | kPa | Joback Method |
| tb | 478.40 | K | Joback Method |
| tc | 701.27 | K | Joback Method |
| tf | 221.10 | K | Joback Method |
| vc | 0.460 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 236.88 | J/molxK | 478.40 | Joback Method |
| cpg | 248.67 | J/molxK | 515.55 | Joback Method |
| cpg | 259.83 | J/molxK | 552.69 | Joback Method |
| cpg | 270.40 | J/molxK | 589.84 | Joback Method |
| cpg | 280.37 | J/molxK | 626.98 | Joback Method |
| cpg | 289.77 | J/molxK | 664.13 | Joback Method |
| cpg | 298.61 | J/molxK | 701.27 | 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=C14044689&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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