

4-Mercaptopentane-2-ol

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|-----------------------------|---|
| Inchi: | InChI=1S/C5H12OS/c1-4(6)3-5(2)7/h4-7H,3H2,1-2H3 |
| InchiKey: | AKFMLHKPSQIJJW-UHFFFAOYSA-N |
| Formula: | C5H12OS |
| SMILES: | CC(O)CC(C)S |
| Mol. weight [g/mol]: | 120.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -121.09 | kJ/mol | Joback Method |
| hf | -270.84 | kJ/mol | Joback Method |
| hfus | 9.79 | kJ/mol | Joback Method |
| hvap | 49.36 | kJ/mol | Joback Method |
| log10ws | -1.47 | | Crippen Method |
| logp | 1.076 | | Crippen Method |
| mcvol | 103.530 | ml/mol | McGowan Method |
| pc | 4294.29 | kPa | Joback Method |
| rinpola | 926.00 | | NIST Webbook |
| tb | 467.96 | K | Joback Method |
| tc | 658.24 | K | Joback Method |
| tf | 213.39 | K | Joback Method |
| vc | 0.377 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 212.56 | J/mol×K | 467.96 | Joback Method |
| cpg | 222.02 | J/mol×K | 499.67 | Joback Method |
| cpg | 231.06 | J/mol×K | 531.39 | Joback Method |
| cpg | 239.68 | J/mol×K | 563.10 | Joback Method |
| cpg | 247.90 | J/mol×K | 594.82 | Joback Method |
| cpg | 255.72 | J/mol×K | 626.53 | Joback Method |
| cpg | 263.16 | J/mol×K | 658.24 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R611879&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

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

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