

Chloromethylmethyl sulfide

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| Other names: | CH3SCH2Cl Methane, chloro(methylthio)- «alpha»-Chlorodimethyl sulfide Chlorodimethyl thioether Chloromethyl methyl thioether Methylthiomethyl chloride Monochlorodimethyl sulfide Sulfide, chloromethyl methyl Chlorodimethyl sulfide Clorodimetilsolfuro Chloro(methylthio)methane NSC 63205 chloromethyl methyl sulphide |
| Inchi: | InChI=1S/C2H5ClS/c1-4-2-3/h2H2,1H3 |
| InchiKey: | JWMLCCRPDOIBAV-UHFFFAOYSA-N |
| Formula: | C2H5ClS |
| SMILES: | CSCCI |
| Mol. weight [g/mol]: | 96.58 |
| CAS: | 2373-51-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -12.85 | kJ/mol | Joback Method |
| hf | -58.48 | kJ/mol | Joback Method |
| hfus | 9.26 | kJ/mol | Joback Method |
| hvap | 31.25 | kJ/mol | Joback Method |
| ie | 9.17 | eV | NIST Webbook |
| log10ws | -1.19 | | Crippen Method |
| logp | 1.546 | | Crippen Method |
| mcvol | 67.630 | ml/mol | McGowan Method |
| pc | 4890.21 | kPa | Joback Method |
| rinpol | 713.00 | | NIST Webbook |
| rinpol | 713.00 | | NIST Webbook |
| tb | 378.20 | K | NIST Webbook |
| tc | 553.87 | K | Joback Method |
| tf | 176.62 | K | Joback Method |
| vc | 0.251 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 93.77 | J/mol×K | 351.37 | Joback Method |
| cpg | 98.65 | J/mol×K | 385.12 | Joback Method |
| cpg | 103.36 | J/mol×K | 418.87 | Joback Method |
| cpg | 107.91 | J/mol×K | 452.62 | Joback Method |
| cpg | 112.29 | J/mol×K | 486.37 | Joback Method |
| cpg | 116.51 | J/mol×K | 520.12 | Joback Method |
| cpg | 120.55 | J/mol×K | 553.87 | 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=C2373515&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 |
| ie: | Ionization energy |
| 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

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