

Carbamodithioic acid, dimethyl-, methyl ester

| | |
|-----------------------------|---|
| Other names: | Carbamic acid, dimethyldithio-, methyl ester Cystogon Forbiat Methyl dimethyldithiocarbamate Methyl N,N-dimethyldithiocarbamate Dimethyldithiocarbamic acid methyl ester |
| Inchi: | InChI=1S/C4H9NS2/c1-5(2)4(6)7-3/h1-3H3 |
| InchiKey: | NBBZMDUHKWRYSZ-UHFFFAOYSA-N |
| Formula: | C4H9NS2 |
| SMILES: | CSC(=S)N(C)C |
| Mol. weight [g/mol]: | 135.25 |
| CAS: | 3735-92-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|----------------------|----------------|
| chs | -3991.00 | kJ/mol | NIST Webbook |
| gf | 243.76 | kJ/mol | Joback Method |
| hf | 130.01 | kJ/mol | Joback Method |
| hfs | -66.90 | kJ/mol | NIST Webbook |
| hfus | 17.87 | kJ/mol | Joback Method |
| hvap | 40.09 | kJ/mol | Joback Method |
| ie | 8.01 | eV | NIST Webbook |
| ie | 8.01 ± 0.03 | eV | NIST Webbook |
| log10ws | -1.30 | | Crippen Method |
| logp | 1.196 | | Crippen Method |
| mcvol | 105.600 | ml/mol | McGowan Method |
| pc | 4474.22 | kPa | Joback Method |
| rinpol | 1082.00 | | NIST Webbook |
| rinpol | 1082.00 | | NIST Webbook |
| ripol | 2012.00 | | NIST Webbook |
| ripol | 2012.00 | | NIST Webbook |
| tb | 442.18 | K | Joback Method |
| tc | 663.52 | K | Joback Method |
| tf | 235.98 | K | Joback Method |
| vc | 0.367 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 189.92 | J/mol×K | 442.18 | Joback Method |
| cpg | 199.76 | J/mol×K | 479.07 | Joback Method |
| cpg | 208.90 | J/mol×K | 515.96 | Joback Method |
| cpg | 217.38 | J/mol×K | 552.85 | Joback Method |
| cpg | 225.25 | J/mol×K | 589.74 | Joback Method |
| cpg | 232.56 | J/mol×K | 626.63 | Joback Method |
| cpg | 239.35 | J/mol×K | 663.52 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C3735920&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|--|
| chs: | Standard solid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfs: | Solid phase 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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/28-071-2/Carbamodithioic-acid-dimethyl-methyl-ester.pdf>

Generated by Cheméo on 2024-04-27 21:58:33.758269357 +0000 UTC m=+16544362.678846679.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.