

DL-Cystine

| | |
|-----------------------------|--|
| Other names: | Cystine, DL- |
| Inchi: | InChI=1S/C6H12N2O4S2/c7-3(5(9)10)1-13-14-2-4(8)6(11)12/h3-4H,1-2,7-8H2,(H,9,10)(H,11,12) |
| InchiKey: | LEVWYRKDKASIDU-UHFFFAOYSA-N |
| Formula: | C6H12N2O4S2 |
| SMILES: | NC(CSSCC(N)C(=O)O)C(=O)O |
| Mol. weight [g/mol]: | 240.30 |
| CAS: | 923-32-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -337.58 | kJ/mol | Joback Method |
| hf | -556.03 | kJ/mol | Joback Method |
| hfus | 34.28 | kJ/mol | Joback Method |
| hvap | 109.94 | kJ/mol | Joback Method |
| log10ws | -0.38 | | Crippen Method |
| logp | -0.808 | | Crippen Method |
| mcvol | 162.940 | ml/mol | McGowan Method |
| pc | 5739.21 | kPa | Joback Method |
| tb | 910.52 | K | Joback Method |
| tc | 1133.18 | K | Joback Method |
| tf | 584.20 | K | Joback Method |
| vc | 0.576 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 458.08 | J/molxK | 910.52 | Joback Method |
| cpg | 463.72 | J/molxK | 947.63 | Joback Method |
| cpg | 468.63 | J/molxK | 984.74 | Joback Method |
| cpg | 472.85 | J/molxK | 1021.85 | Joback Method |
| cpg | 476.36 | J/molxK | 1058.96 | Joback Method |
| cpg | 479.17 | J/molxK | 1096.07 | Joback Method |
| cpg | 481.31 | J/molxK | 1133.18 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.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=C923320&Units=SI |

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 |
| h vap: | 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 |

Latest version available from:

<https://www.cheméo.com/cid/64-054-1/DL-Cystine.pdf>

Generated by Cheméo on 2024-05-02 08:19:55.901177153 +0000 UTC m=+16927244.821754469.

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