

Butanedioic acid, mercapto-

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|-----------------------------|---|
| Other names: | 2-Mercaptosuccinic acid 2-Sulfanylsuccinic acid 2-Thiomalic acid Butanedioic acid, 2-mercapto- Malic acid, 2-thio- Mercaptosuccinic acid Monomercaptosuccinic acid NSC 7302 Thiomalic acid USAF EK-P-6297 USAF M-2 succinic acid, mercapto- «alpha»-Mercaptosuccinic acid |
| Inchi: | InChI=1S/C4H6O4S/c5-3(6)1-2(9)4(7)8/h2,9H,1H2,(H,5,6)(H,7,8) |
| InchiKey: | NJRXVEJTAYWCQJ-UHFFFAOYSA-N |
| Formula: | C4H6O4S |
| SMILES: | O=C(O)CC(S)C(=O)O |
| Mol. weight [g/mol]: | 150.15 |
| CAS: | 70-49-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -521.73 | kJ/mol | Joback Method |
| hf | -622.31 | kJ/mol | Joback Method |
| hfus | 18.01 | kJ/mol | Joback Method |
| hvap | 77.70 | kJ/mol | Joback Method |
| log10ws | 0.12 | | Crippen Method |
| logp | -0.156 | | Crippen Method |
| mcvol | 98.450 | ml/mol | McGowan Method |
| pc | 6718.62 | kPa | Joback Method |
| tb | 645.44 | K | Joback Method |
| tc | 839.92 | K | Joback Method |
| tf | 377.80 | K | Joback Method |
| vc | 0.357 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 225.07 | J/molxK | 645.44 | Joback Method |
| cpg | 230.40 | J/molxK | 677.85 | Joback Method |
| cpg | 235.39 | J/molxK | 710.27 | Joback Method |
| cpg | 240.07 | J/molxK | 742.68 | Joback Method |
| cpg | 244.44 | J/molxK | 775.10 | Joback Method |
| cpg | 248.51 | J/molxK | 807.51 | Joback Method |
| cpg | 252.29 | J/molxK | 839.92 | Joback Method |

Sources

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|---|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C70495&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Thermodynamics of solubility of thiomalic acid in different organic solvents | https://www.doi.org/10.1016/j.fluid.2013.05.002 |
| The solubility of mercaptosuccinic acid in water+ (methanol, ethanol, acetone) mixtures from 278.15 to 333.15 K | https://www.doi.org/10.1016/j.fluid.2013.11.001 |
| Thermodynamic analysis for solid-liquid equilibrium of mercaptosuccinic acid in binary solvent of methanol and ethyl acetate at temperatures between (278.15 and 333.15) K: | https://www.doi.org/10.1016/j.fluid.2015.02.008 |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |

vc: Critical Volume

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