

val-gly

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| Inchi: | InChI=1S/C7H14N2O3/c1-4(2)6(8)7(12)9-3-5(10)11/h4,6H,3,8H2,1-2H3,(H,9,12)(H,10,11) |
| InchiKey: | IOUPEELXVYPCPG-UHFFFAOYSA-N |
| Formula: | C7H14N2O3 |
| SMILES: | CC(C)C(N)C(=O)NCC(=O)O |
| Mol. weight [g/mol]: | 174.20 |
| CAS: | 686-43-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| basg | 874.10 | kJ/mol | NIST Webbook |
| gf | -235.64 | kJ/mol | Joback Method |
| hf | -488.50 | kJ/mol | Joback Method |
| hfus | 24.42 | kJ/mol | Joback Method |
| hvap | 77.65 | kJ/mol | Joback Method |
| log10ws | -0.12 | | Crippen Method |
| logp | -0.829 | | Crippen Method |
| mvol | 138.460 | ml/mol | McGowan Method |
| pc | 3975.52 | kPa | Joback Method |
| tb | 681.30 | K | Joback Method |
| tc | 876.47 | K | Joback Method |
| tf | 435.25 | K | Joback Method |
| vc | 0.510 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 379.80 | J/molxK | 681.30 | Joback Method |
| cpg | 389.37 | J/molxK | 713.83 | Joback Method |
| cpg | 398.38 | J/molxK | 746.36 | Joback Method |
| cpg | 406.84 | J/molxK | 778.88 | Joback Method |
| cpg | 414.76 | J/molxK | 811.41 | Joback Method |
| cpg | 422.17 | J/molxK | 843.94 | Joback Method |
| cpg | 429.08 | J/molxK | 876.47 | 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=C686431&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| basg: | Gas basicity |
| 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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