# val-ser

**Inchi:** InChI=1S/C8H16N2O4/c1-4(2)6(9)7(12)10-5(3-11)8(13)14/h4-6,11H,3,9H2,1-2H3,(H,10,
**InchiKey:** STTYIMSDIYISRG-UHFFFAOYSA-N
**Formula:** C8H16N2O4
**SMILES:** CC(C)C(N)C(=O)NC(CO)C(=O)O
**Mol. weight [g/mol]:** 204.22
**CAS:** 13588-94-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| basg | 874.10 | kJ/mol | NIST Webbook |
| gf | -366.48 | kJ/mol | Joback Method |
| hf | -666.65 | kJ/mol | Joback Method |
| hfus | 27.58 | kJ/mol | Joback Method |
| hvap | 96.17 | kJ/mol | Joback Method |
| log10ws | 0.09 | | Crippen Method |
| logp | -1.469 | | Crippen Method |
| mcvol | 158.420 | ml/mol | McGowan Method |
| pc | 3995.65 | kPa | Joback Method |
| tb | 795.92 | K | Joback Method |
| tc | 988.60 | K | Joback Method |
| tf | 492.34 | K | Joback Method |
| vc | 0.580 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 476.06 | J/mol×K | 795.92 | Joback Method |
| cpg | 484.71 | J/mol×K | 828.03 | Joback Method |
| cpg | 492.79 | J/mol×K | 860.15 | Joback Method |
| cpg | 500.33 | J/mol×K | 892.26 | Joback Method |
| cpg | 507.34 | J/mol×K | 924.37 | Joback Method |
| cpg | 513.85 | J/mol×K | 956.49 | Joback Method |
| cpg | 519.88 | J/mol×K | 988.60 | 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=C13588948&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |