# Serine, n-(2-imidazolin-2-yl)-

**Inchi:** InChI=1S/C6H11N3O3/c10-3-4(5(11)12)9-6-7-1-2-8-6/h4,10H,1-3H2,(H,11,12)(H2,7,8,9)
**InchiKey:** PVKQQMOUDJKVSX-UHFFFAOYSA-N
**Formula:** C6H11N3O3
**SMILES:** O=C(O)C(CO)NC1=NCCN1
**Mol. weight [g/mol]:** 173.17
**CAS:** 133318-36-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -46.89 | kJ/mol | Joback Method |
| hf | -300.11 | kJ/mol | Joback Method |
| hfus | 31.07 | kJ/mol | Joback Method |
| hvap | 89.59 | kJ/mol | Joback Method |
| log10ws | 0.76 | | Crippen Method |
| logp | -2.019 | | Crippen Method |
| mcvol | 123.490 | ml/mol | McGowan Method |
| pc | 6239.25 | kPa | Joback Method |
| tb | 750.98 | K | Joback Method |
| tc | 955.52 | K | Joback Method |
| tf | 571.60 | K | Joback Method |
| vc | 0.459 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 370.96 | J/mol×K | 750.98 | Joback Method |
| cpg | 379.82 | J/mol×K | 785.07 | Joback Method |
| cpg | 388.02 | J/mol×K | 819.16 | Joback Method |
| cpg | 395.57 | J/mol×K | 853.25 | Joback Method |
| cpg | 402.48 | J/mol×K | 887.34 | Joback Method |
| cpg | 408.75 | J/mol×K | 921.43 | Joback Method |
| cpg | 414.39 | J/mol×K | 955.52 | Joback Method |

# Sources

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|---|---|
| **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=C133318362&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **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 |