

N-Serylserine

Other names:	Serylserine
Inchi:	InChI=1S/C6H12N2O5/c7-3(1-9)5(11)8-4(2-10)6(12)13/h3-4,9-10H,1-2,7H2,(H,8,11)(H,1
InchiKey:	XZKQVQKUZMAADP-UHFFFAOYSA-N
Formula:	C6H12N2O5
SMILES:	NC(CO)C(=O)NC(CO)C(=O)O
Mol. weight [g/mol]:	192.17
CAS:	6620-95-7

Physical Properties

Property code	Value	Unit	Source
basg	886.40	kJ/mol	NIST Webbook
chs	-2898.30 ± 0.30	kJ/mol	NIST Webbook
gf	-517.70	kJ/mol	Joback Method
hf	-772.32	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	108.78	kJ/mol	Joback Method
log10ws	1.42		Crippen Method
logp	-3.132		Crippen Method
mcvol	136.110	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
tb	842.78	K	Joback Method
tc	1036.34	K	Joback Method
tf	545.62	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.68	J/molxK	842.78	Joback Method
cpg	416.88	J/molxK	875.04	Joback Method
cpg	422.63	J/molxK	907.30	Joback Method
cpg	427.96	J/molxK	939.56	Joback Method
cpg	432.88	J/molxK	971.82	Joback Method
cpg	437.41	J/molxK	1004.08	Joback Method

Sources

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=C6620957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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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