

gly-ser

Inchi:	InChI=1S/C5H10N2O4/c6-3(2-8)5(11)7-1-4(9)10/h3,8H,1-2,6H2,(H,7,11)(H,9,10)
InchiKey:	WOUIMBGNEUWXQG-UHFFFAOYSA-N
Formula:	C5H10N2O4
SMILES:	NC(CO)C(=O)NCC(=O)O
Mol. weight [g/mol]:	162.14
CAS:	687-63-8

Physical Properties

Property code	Value	Unit	Source
basg	880.90	kJ/mol	NIST Webbook
gf	-386.86	kJ/mol	Joback Method
hf	-594.17	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	90.26	kJ/mol	Joback Method
log10ws	1.21		Crippen Method
logp	-2.493		Crippen Method
mcvol	116.150	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method
tb	728.16	K	Joback Method
tc	916.83	K	Joback Method
tf	488.53	K	Joback Method
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.34	J/mol×K	728.16	Joback Method
cpg	328.84	J/mol×K	759.60	Joback Method
cpg	334.93	J/mol×K	791.05	Joback Method
cpg	340.63	J/mol×K	822.49	Joback Method
cpg	345.95	J/mol×K	853.94	Joback Method
cpg	350.90	J/mol×K	885.38	Joback Method
cpg	355.50	J/mol×K	916.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C687638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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