val-gly

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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.80	J/mol×K	681.30	Joback Method
cpg	389.37	J/mol×K	713.83	Joback Method
cpg	398.38	J/mol×K	746.36	Joback Method
cpg	406.84	J/mol×K	778.88	Joback Method
cpg	414.76	J/mol×K	811.41	Joback Method
cpg	422.17	J/mol×K	843.94	Joback Method
cpg	429.08	J/mol×K	876.47	Joback Method

Sources

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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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