

dl-Alanyl-dl-valine

Other names:	Alanylvaline (DL)
Inchi:	InChI=1S/C8H16N2O3/c1-4(2)6(8(12)13)10-7(11)5(3)9/h4-6H,9H2,1-3H3,(H,10,11)(H,12)
InchiKey:	LIWMQSWFLXEGMA-UHFFFAOYSA-N
Formula:	C8H16N2O3
SMILES:	CC(N)C(=O)NC(C(=O)O)C(C)C
Mol. weight [g/mol]:	188.22
CAS:	1999-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-229.66	kJ/mol	Joback Method
hf	-514.42	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	-0.441		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	703.74	K	Joback Method
tc	900.15	K	Joback Method
tf	431.52	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.26	J/molxK	867.42	Joback Method
cpg	430.34	J/molxK	703.74	Joback Method
cpg	440.75	J/molxK	736.48	Joback Method
cpg	450.52	J/molxK	769.21	Joback Method
cpg	459.68	J/molxK	801.95	Joback Method
cpg	468.26	J/molxK	834.68	Joback Method
cpg	483.71	J/molxK	900.15	Joback Method
cps	240.00	J/molxK	298.00	NIST Webbook

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=C1999468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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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