

L-valine, n-acetyl-

Other names:	Valine, N-acetyl-, L-Acetylvaline N-Acetyl-L-valine N-Acetylvaline
Inchi:	InChI=1S/C7H13NO3/c1-4(2)6(7(10)11)8-5(3)9/h4,6H,1-3H3,(H,8,9)(H,10,11)
InchiKey:	IHYJTAOFMMMOPX-UHFFFAOYSA-N
Formula:	C7H13NO3
SMILES:	CC(=O)NC(C(=O)O)C(C)C
Mol. weight [g/mol]:	159.19

Physical Properties

Property code	Value	Unit	Source
hfus	19.23	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-0.71		Cheméo Relay (1.0)
logp	0.232		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
tf	429.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.77	J/mol×K	608.77	Joback Method
cpg	335.59	J/mol×K	639.95	Joback Method
cpg	344.89	J/mol×K	671.14	Joback Method
cpg	353.70	J/mol×K	702.32	Joback Method
cpg	362.02	J/mol×K	733.50	Joback Method
cpg	369.86	J/mol×K	764.68	Joback Method
cpg	377.24	J/mol×K	795.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96811&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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