N-Acetyl L-valinamide

Inchi: InChI=1S/C7H14N2O2/c1-4(2)6(7(8)11)9-5(3)10/h4,6H,1-3H3,(H2,8,11)(H,9,10)
InchiKey: WEHJKQHCMGQEEF-UHFFFAOYSA-N
Formula: C7H14N2O2
SMILES: CC(=O)NC(C(N)=O)C(C)C
Mol. weight [g/mol]: 158.20
CAS: 37933-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-98.82	kJ/mol	Joback Method
hf	-336.27	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hsub	133.10 ± 2.20	kJ/mol	NIST Webbook
hvap	60.97	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	-0.368		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	589.12	K	Joback Method
tc	796.38	K	Joback Method
tf	509.00 ± 0.40	K	NIST Webbook
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.68	J/mol×K	589.12	Joback Method
cpg	344.36	J/mol×K	623.66	Joback Method
cpg	355.37	J/mol×K	658.21	Joback Method
cpg	365.74	J/mol×K	692.75	Joback Method
cpg	375.48	J/mol×K	727.30	Joback Method
cpg	384.60	J/mol×K	761.84	Joback Method
cpg	393.14	J/mol×K	796.38	Joback Method
hfust	39.10	kJ/mol	509.00	NIST Webbook

hsubt	129.80 ± 1.90	kJ/mol	376.00	NIST Webbook
hsubt	126.00 ± 2.00	kJ/mol	408.00	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=C37933883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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