2-(Acetylamino)-N-methylpropanamide(L)

Inchi: InChI=1S/C6H12N2O2/c1-4(6(10)7-3)8-5(2)9/h4H,1-3H3,(H,7,10)(H,8,9)/t4-/m1/s1
InchiKey: VHCVPWSUVMHJLL-SCSAIBSYSA-N
Formula: C6H12N2O2
SMILES: CNC(=O)C(C)NC(C)=O
Mol. weight [g/mol]: 144.17
CAS: 19701-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-81.86	kJ/mol	Joback Method
hf	-290.67	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.743		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	544.32	K	Joback Method
tc	742.19	K	Joback Method
tf	347.56	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.87	J/mol×K	544.32	Joback Method
cpg	288.60	J/mol×K	577.30	Joback Method
cpg	298.76	J/mol×K	610.28	Joback Method
cpg	308.38	J/mol×K	643.25	Joback Method
cpg	317.47	J/mol×K	676.23	Joback Method
cpg	326.04	J/mol×K	709.21	Joback Method
cpg	334.10	J/mol×K	742.19	Joback Method
cps	201.30	J/mol×K	298.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19701838&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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