(3S)-(-)-3-Acetamidopyrrolidine

Inchi: InChI=1S/C6H12N2O/c1-5(9)8-6-2-3-7-4-6/h6-7H,2-4H2,1H3,(H,8,9)/t6-/m0/s1
InchiKey: HDCCJUCOIKLZNM-LURJTMIESA-N
Formula: C6H12N2O
SMILES: CC(=O)NC1CCNC1
Mol. weight [g/mol]: 128.17
CAS: 79286-74-1

Physical Properties

Property code	Value	Unit	Source
gf	84.37	kJ/mol	Joback Method
hf	-127.99	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	-0.516		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	504.55	K	Joback Method
tc	723.58	K	Joback Method
tf	375.90	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.67	J/mol×K	504.55	Joback Method
cpg	254.49	J/mol×K	541.05	Joback Method
cpg	267.55	J/mol×K	577.56	Joback Method
cpg	279.86	J/mol×K	614.06	Joback Method
cpg	291.44	J/mol×K	650.57	Joback Method
cpg	302.32	J/mol×K	687.07	Joback Method
cpg	312.50	J/mol×K	723.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79286741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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