2-Azetidinecarboxylic acid

Other names: L-pyrrolidine-2-carboxylic acid
Inchi: InChI=1S/C4H7NO2/c6-4(7)3-1-2-5-3/h3,5H,1-2H2,(H,6,7)
InchiKey: IADUEWIQBXOCDZ-UHFFFAOYSA-N
Formula: C4H7NO2
SMILES: O=C(O)C1CCN1
Mol. weight [g/mol]: 101.10
CAS: 2517-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-146.58	kJ/mol	Joback Method
hf	-286.25	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	-0.567		Crippen Method
mcvol	73.780	ml/mol	McGowan Method
pc	6229.41	kPa	Joback Method
tb	496.53	K	Joback Method
tc	698.30	K	Joback Method
tf	365.04	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.96	J/mol×K	496.53	Joback Method
cpg	169.32	J/mol×K	530.16	Joback Method
cpg	177.23	J/mol×K	563.79	Joback Method
cpg	184.70	J/mol×K	597.42	Joback Method
cpg	191.75	J/mol×K	631.05	Joback Method
cpg	198.39	J/mol×K	664.68	Joback Method
cpg	204.65	J/mol×K	698.30	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=C2517046&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