Pipecolamide

Inchi: InChI=1S/C6H12N2O/c7-6(9)5-3-1-2-4-8-5/h5,8H,1-4H2,(H2,7,9)
InchiKey: XIMBESZRBTVIOD-UHFFFAOYSA-N
Formula: C6H12N2O
SMILES: N=C(O)C1CCCCN1
Mol. weight [g/mol]: 128.17
CAS: 19889-77-1

Physical Properties

Property code	Value	Unit	Source
gf	178.58	kJ/mol	Joback Method
hf	-28.94	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	0.664		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
tb	581.30	K	Joback Method
tf	399.39	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.22	J/mol×K	581.30	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method
cpg	10.49	J/mol×K	100.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19889771&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point