Nipecotamide

Other names: 3-piperidinecarboxamide
piperidine-3-carboxamide
Inchi: InChI=1S/C6H12N2O/c7-6(9)5-2-1-3-8-4-5/h5,8H,1-4H2,(H2,7,9)
InchiKey: BVOCPVIXARZNQN-UHFFFAOYSA-N
Formula: C6H12N2O
SMILES: N=C(O)C1CCCNC1
Mol. weight [g/mol]: 128.17
CAS: 4138-26-5

Physical Properties

Property code	Value	Unit	Source
gf	178.58	kJ/mol	Joback Method
hf	-28.94	kJ/mol	Joback Method
hsub	112.50 ± 1.30	kJ/mol	NIST Webbook
hvap	64.90	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	0.521		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

hvapt	112.50	kJ/mol	386.00	Thermochemical study of 1-, 3- and 4-piperidinecarboxamide derivatives

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4138265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study of 1-, 3- and 4-piperidinecarboxamide derivatives:	https://www.doi.org/10.1016/j.tca.2006.11.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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