Piperidine-4-carbonitrile

Other names: 4-Cyanopiperidine
Inchi: InChI=1S/C6H10N2/c7-5-6-1-3-8-4-2-6/h6,8H,1-4H2
InchiKey: FSDNTQSJGHSJBG-UHFFFAOYSA-N
Formula: C6H10N2
SMILES: N#CC1CCNCC1
Mol. weight [g/mol]: 110.16
CAS: 4395-98-6

Physical Properties

Property code	Value	Unit	Source
affp	912.30	kJ/mol	NIST Webbook
basg	879.20	kJ/mol	NIST Webbook
gf	244.98	kJ/mol	Joback Method
hf	89.84	kJ/mol	Joback Method
hfus	14.23	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.510		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	506.86	K	Joback Method
tc	743.63	K	Joback Method
tf	334.78	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.60	J/mol×K	506.86	Joback Method
cpg	220.83	J/mol×K	546.32	Joback Method
cpg	233.31	J/mol×K	585.78	Joback Method
cpg	245.04	J/mol×K	625.24	Joback Method
cpg	256.04	J/mol×K	664.71	Joback Method
cpg	266.33	J/mol×K	704.17	Joback Method

cpg	275.90	J/mol×K	743.63	Joback Method

Sources

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=C4395986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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