1-Piperidineacetonitrile

Other names:	1-Piperidinoacetonitrile
	Acetonitrile, piperidino-
	N-Piperidinoacetonitrile
	Piperidinoacetonitrile
	Piperidoacetonitrile
	N-Cyanomethylpiperidine
	piperidine-1-acetonitrile
Inchi:	InChI=1S/C7H12N2/c8-4-7-9-5-2-1-3-6-9/h1-3,5-7H2
InchiKey:	CLVBVRODHJFTGF-UHFFFAOYSA-N
Formula:	C7H12N2
SMILES:	N#CCN1CCCCC1
Mol. weight [g/mol]:	124.18
CAS:	3010-03-5

Physical Properties

Property code	Value	Unit	Source
chs	-4478.90 ± 1.00	kJ/mol	NIST Webbook
hf	83.00 ± 1.20	kJ/mol	NIST Webbook
hfs	9.40 ± 1.10	kJ/mol	NIST Webbook
hsub	56.02 ± 0.49	kJ/mol	NIST Webbook
log10ws	-1.08		Crippen Method
logp	0.996		Crippen Method
mcvol	109.990	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.57	kJ/mol	293.20	NIST Webbook
hvapt	56.00 ± 0.50	kJ/mol	320.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3010035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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