Cyclohexanecarbonitrile, 1-(1-piperidinyl)-

Other names:	Cyclohexanecarbonitrile, 1-piperidino-
	1-Piperidinocyclohexanecarbonitrile
	1-(1-Cyanocyclohexyl)piperidine
	PCC
	Piperidinocyclohexanecarbonitrile
Inchi:	InChI=1S/C12H20N2/c13-11-12(7-3-1-4-8-12)14-9-5-2-6-10-14/h1-10H2
InchiKey:	WWSAYKJWUZJLRT-UHFFFAOYSA-N
Formula:	C12H20N2
SMILES:	N#CC1(N2CCCCC2)CCCCC1
Mol. weight [g/mol]:	192.30
CAS:	3867-15-0

Physical Properties

Property code	Value	Unit	Source
chs	-7496.18 ± 0.37	kJ/mol	NIST Webbook
hf	3.53 ± 0.77	kJ/mol	NIST Webbook
hfs	-84.23 ± 0.44	kJ/mol	NIST Webbook
hsub	87.80 ± 0.60	kJ/mol	NIST Webbook
hsub	87.76 ± 0.63	kJ/mol	NIST Webbook
hsub	87.80	kJ/mol	NIST Webbook
log10ws	-3.18		Crippen Method
logp	2.699		Crippen Method
mcvol	169.580	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.44	kJ/mol	339.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3867150&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume