Piperidine, 1-(cyanoacetyl)-

Other names:	1-Cyanoacetylpiperidine
	N-(2-Cyanoacetyl)piperidine
Inchi:	InChI=1S/C8H12N2O/c9-5-4-8(11)10-6-2-1-3-7-10/h1-4,6-7H2
InchiKey:	ANLQHFYDQPMDJY-UHFFFAOYSA-N
Formula:	C8H12N2O
SMILES:	N#CCC(=O)N1CCCCC1
Mol. weight [g/mol]:	152.19
CAS:	15029-30-8

Physical Properties

Property code	Value	Unit	Source
hsub	103.50 ± 1.90	kJ/mol	NIST Webbook
log10ws	-1.28		Crippen Method
logp	0.913		Crippen Method
mcvol	125.650	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15029308&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

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

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