

# Piperidine, 1-(cyanoacetyl)-

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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15029308&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15029308&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/97-078-9/Piperidine-1-cyanoacetyl.pdf>

Generated by Cheméo on 2024-04-30 09:24:03.678555952 +0000 UTC m=+16758292.599133275.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.