

Pyrrolidine, 1-(1-cyclohexen-1-yl)-

Other names:	Cyclohexanone pyrrolidine enamine
	N-(1-Cyclohexen-1-yl)pyrrolidine
	N-(1-Cyclohexenyl)pyrrolidine
	1-(1-Cyclohexen-1-yl)pyrrolidine
	1-(1-Pyrrolidino)-1-cyclohexene
	1-(1-Pyrrolidinyl)cyclohexene
	1-Pyrrolidino-1-cyclohexene
	1-Pyrrolidinocyclohexene
	1-Pyrrolidinyl-1-cyclohexene
	1-(Cyclohexen-1-yl)pyrrolidine
	N-Pyrrolidino-1-cyclohexene
	1-(1-Cyclohexenyl)pyrrolidine
	NSC 29652
	N-(cyclohex-1-en-1-yl)pyrrolidine
Inchi:	InChI=1S/C10H17N/c1-2-6-10(7-3-1)11-8-4-5-9-11/h6H,1-5,7-9H2
InchiKey:	KTZNVZJECQAMBV-UHFFFAOYSA-N
Formula:	C10H17N
SMILES:	C1=C(N2CCCC2)CCCC1
Mol. weight [g/mol]:	151.25
CAS:	1125-99-1

Physical Properties

Property code	Value	Unit	Source
ie	7.14 ± 0.05	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.10 ± 0.03	eV	NIST Webbook
log10ws	-2.72		Crippen Method
logp	2.540		Crippen Method
mcvol	135.720	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	2.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1125991&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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