1H-Pyrrolizine, hexahydro-

Other names:	Hexahydropyrrolizine
	Pyrrolizidine
	1-Azabicyclo[3.3.0]octane
Inchi:	InChI=1S/C7H13N/c1-3-7-4-2-6-8(7)5-1/h7H,1-6H2
InchiKey:	ADRDEXBBJTUCND-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	C1CC2CCCN2C1
Mol. weight [g/mol]:	111.18
CAS:	643-20-9

Physical Properties

Property code	Value	Unit	Source
chl	-4564.20 ± 3.00	kJ/mol	NIST Webbook
hf	-3.90	kJ/mol	NIST Webbook
hfl	-48.30 ± 3.10	kJ/mol	NIST Webbook
hvap	44.40	kJ/mol	NIST Webbook
hvap	44.40	kJ/mol	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.245		Crippen Method
mcvol	97.750	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C643209&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume