

1-METHYL-1,4-DIAZACYCLOHEPTANE

Other names:	1H-1,4-Diazepine, hexahydro-1-methyl-
Inchi:	InChI=1S/C6H14N2/c1-8-5-2-3-7-4-6-8/h7H,2-6H2,1H3
InchiKey:	FXHRAKUEZPSMLJ-UHFFFAOYSA-N
Formula:	C6H14N2
SMILES:	CN1CCCNCC1
Mol. weight [g/mol]:	114.19

Physical Properties

Property code	Value	Unit	Source
hvap	55.96	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	1.64		Cheméo Relay (1.0)
logp	-0.088		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
tb	427.52	K	Cheméo Relay (1.0)
tf	239.96	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4318370&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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