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