1-Azabicyclo[2.2.1]heptane

Inchi: InChI=1S/C6H11N/c1-3-7-4-2-6(1)5-7/h6H,1-5H2
InchiKey: JVCBVWTTXCNJBJ-UHFFFAOYSA-N
Formula: C6H11N
SMILES: C1CN2CCC1C2
Mol. weight [g/mol]: 97.16

Physical Properties

Property code	Value	Unit	Source
hf	39.82	kJ/mol	Cheméo Relay (1.0)
ie	7.73	eV	Cheméo Relay (1.0)
logp	0.712		Crippen Method
mcvol	83.660	ml/mol	McGowan Method
tb	403.00	K	NIST Webbook
tf	351.50 ± 0.50	K	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C279276&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

hf: Enthalpy of formation at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point