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
CAS: 279-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.45		Crippen Method
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
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

Legend

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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