

2,3-Diazabicyclo[2.2.1]heptane,2,3-dimethyl-,(2-en

Inchi: InChI=1S/C7H14N2/c1-8-6-3-4-7(5-6)9(8)2/h6-7H,3-5H2,1-2H3
InchiKey: VAUNORIQTFNCKC-UHFFFAOYSA-N
Formula: C7H14N2
SMILES: CN1C2CCC(C2)N1C
Mol. weight [g/mol]: 126.20
CAS: 53798-46-2

Physical Properties

Property code	Value	Unit	Source
ie	7.66	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	0.700		Crippen Method
mcvol	107.730	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53798462&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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