3,7-Diazabicyclo[3.3.1]nonane, 3,7-dimethyl-

Inchi: InChI=1S/C9H18N2/c1-10-4-8-3-9(5-10)7-11(2)6-8/h8-9H,3-7H2,1-2H3
InchiKey: XVHVEMJNJDESBO-UHFFFAOYSA-N
Formula: C9H18N2
SMILES: CN1CC2CC(C1)CN(C)C2
Mol. weight [g/mol]: 154.25
CAS: 14789-33-4

Physical Properties

Property code	Value	Unit	Source
ie	6.80	eV	NIST Webbook
ie	7.84	eV	NIST Webbook
log10ws	-0.04		Crippen Method
logp	0.500		Crippen Method
mcvol	135.910	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14789334&Units=SI

Legend

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