

2,3-Diazabicyclo[2.2.2]octane,1,2,3,4-tetramethyl-

Inchi: InChI=1S/C10H20N2/c1-9-5-7-10(2,8-6-9)12(4)11(9)3/h5-8H2,1-4H3/t9-,10-
InchiKey: DVEROZLVUXLTFB-MGCOHNPYSA-N
Formula: C10H20N2
SMILES: CN1N(C)C2(C)CCC1(C)CC2
Mol. weight [g/mol]: 168.28
CAS: 53779-86-5

Physical Properties

Property code	Value	Unit	Source
ie	7.43	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	1.870		Crippen Method
mcvol	150.000	ml/mol	McGowan Method

Sources

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=C53779865&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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