2,3-Diazabicyclo[2.2.2]octane,2,3-dimethyl-,trans-

Inchi: InChI=1S/C8H16N2/c1-9-7-3-5-8(6-4-7)10(9)2/h7-8H,3-6H2,1-2H3/t7-,8-
InchiKey: HIWDJUZJJXARGW-ZKCHVHJHSA-N
Formula: C8H16N2
SMILES: CN1C2CCC(CC2)N1C
Mol. weight [g/mol]: 140.23
CAS: 53779-85-4

Physical Properties

Property code	Value	Unit	Source
ie	7.46	eV	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.090		Crippen Method
mcvol	121.820	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=C53779854&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.