1,5-diazabicyclo[4.4.0]dec-6-ene (DBD)

Inchi: InChI=1S/C8H14N2/c1-2-6-10-7-3-5-9-8(10)4-1/h4,9H,1-3,5-7H2
InchiKey: ADYDYSSRJIVQDA-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: C1=C2NCCCN2CCC1
Mol. weight [g/mol]: 138.21
CAS: 19616-52-5

Physical Properties

Property code	Value	Unit	Source
affp	1046.40	kJ/mol	NIST Webbook
basg	1014.00	kJ/mol	NIST Webbook
log10ws	-1.56		Crippen Method
logp	0.917		Crippen Method
mcvol	117.520	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19616525&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume