7-isopropyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ITBD)

Inchi: InChI=1S/C10H19N3/c1-9(2)13-8-4-7-12-6-3-5-11-10(12)13/h9H,3-8H2,1-2H3
InchiKey: INNBYWMGBODUGY-UHFFFAOYSA-N
Formula: C10H19N3
SMILES: CC(C)N1CCCN2CCCN=C21
Mol. weight [g/mol]: 181.28
CAS: 160172-95-2

Physical Properties

Property code	Value	Unit	Source
affp	1071.60	kJ/mol	NIST Webbook
basg	1039.20	kJ/mol	NIST Webbook
log10ws	-1.20		Crippen Method
logp	1.162		Crippen Method
mcvol	155.680	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=C160172952&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

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