7-ethyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ETBD)

Inchi: InChI=1S/C9H17N3/c1-2-11-7-4-8-12-6-3-5-10-9(11)12/h2-8H2,1H3
InchiKey: AAPJUEKLMYSSCH-UHFFFAOYSA-N
Formula: C9H17N3
SMILES: CCN1CCCN2CCCN=C12
Mol. weight [g/mol]: 167.25
CAS: 95510-44-4

Physical Properties

Property code	Value	Unit	Source
affp	1068.20	kJ/mol	NIST Webbook
basg	1035.80	kJ/mol	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.774		Crippen Method
mcvol	141.590	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=C95510444&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