2H-Pyrimido[1,2-a]pyrimidine, 1,3,4,6,7,8-hexahydro-

Other names: 1,3,4,6,7,8-Hexahydro-2H-pyrimido[1,2-a]pyrimidine
1,5,7-Triazabicyclo [4.4.0]dec-5-ene
Inchi: InChI=1S/C7H13N3/c1-3-8-7-9-4-2-6-10(7)5-1/h1-6H2,(H,8,9)
InchiKey: FVKFHMNJTHKMRX-UHFFFAOYSA-N
Formula: C7H13N3
SMILES: C1CN=C2NCCCN2C1
Mol. weight [g/mol]: 139.20
CAS: 5807-14-7

Physical Properties

Property code	Value	Unit	Source
affp	1054.60	kJ/mol	NIST Webbook
basg	1022.10	kJ/mol	NIST Webbook
log10ws	-0.46		Crippen Method
logp	0.041		Crippen Method
mcvol	113.410	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5807147&Units=SI
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

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