1-H-Azepine, hexahydro-1-phenyl

Inchi: InChI=1S/C12H17N/c1-2-7-11-13(10-6-1)12-8-4-3-5-9-12/h3-5,8-9H,1-2,6-7,10-11H2
InchiKey: YMDZJGQBSPNMEF-UHFFFAOYSA-N
Formula: C12H17N
SMILES: c1ccc(N2CCCCCC2)cc1
Mol. weight [g/mol]: 175.27
CAS: 40832-99-3

Physical Properties

Property code	Value	Unit	Source
affp	956.60	kJ/mol	NIST Webbook
basg	925.80	kJ/mol	NIST Webbook
log10ws	-2.95		Crippen Method
logp	3.067		Crippen Method
mcvol	155.300	ml/mol	McGowan Method

Sources

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=C40832993&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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