

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

Other names: 1,3,4,6,7,8-Hexahydro-1-methyl-2H-pyrimido(1,2-a)pyrimidine
7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene

Inchi: InChI=1S/C8H15N3/c1-10-5-3-7-11-6-2-4-9-8(10)11/h2-7H2,1H3

InchiKey: OEBXWWBYZJNKRK-UHFFFAOYSA-N

Formula: C8H15N3

SMILES: CN1CCCN2CCCN=C12

Mol. weight [g/mol]: 153.22

CAS: 84030-20-6

Physical Properties

Property code	Value	Unit	Source
affp	1062.70	kJ/mol	NIST Webbook
basg	1030.20	kJ/mol	NIST Webbook
log10ws	-0.26		Crippen Method
logp	0.384		Crippen Method
mcvol	127.500	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C84030206&Units=SI>

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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