

PSILOCYBIN

Other names:	1H-Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate
	1H-Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate (ester)
	3-(2-(Dimethylamino)ethyl)-1H-indol-4-ol dihydrogen phosphate ester
	3-2'-Dimethylaminoethylindol-4-phosphate
	3-[2-(Dimethylamino)ethyl]indol-4-ol dihydrogen phosphate ester
	3-[2-(Dimethylamino)ethyl]indol-4-yl dihydrogen phosphate
	4-Phosphoryloxy-N,N-dimethyltryptamine
	Cy 39
	Indocybin
	Indol-4-ol, 3-(2-(dimethylamino)ethyl)-, dihydrogen phosphate
	Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate (ester)
	O-Phosphoryl-4-hydroxy-N,N-dimethyltryptamine
	Psilocibin
	Psilocin phosphate ester
	Psilocybin
	Psilotsibin
	Psylocybin
	Teonanacatl
Inchi:	InChI=1S/C12H17N2O4P/c1-14(2)7-6-9-8-13-10-4-3-5-11(12(9)10)18-19(15,16)17/h3-5,8,11,12,14,15,16,17,19
InchiKey:	QVDSEJDULKHCG-UHFFFAOYSA-N
Formula:	C12H17N2O4P
SMILES:	CN(C)CCc1c[nH]c2cccc(OP(=O)(O)O)c12
Mol. weight [g/mol]:	284.25

Physical Properties

Property code	Value	Unit	Source
ie	8.12	eV	Cheméo Relay (1.0)
logp	1.262		Crippen Method
mccvol	204.920	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C520525&Units=SI>

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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