

Psilocybine

Other names:

Psilocybin
1H-Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate (ester)
Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate (ester)
Cy 39
Indocybin
3-[2-(Dimethylamino)ethyl]indol-4-ol dihydrogen phosphate ester
3-[2-(Dimethylamino)ethyl]indol-4-yl dihydrogen phosphate
1H-Indol-4-ol, 3-[2-(dimethylamino)ethyl]-, dihydrogen phosphate
Indol-4-ol, 3-(2-(dimethylamino)ethyl)-, dihydrogen phosphate
3-(2-(Dimethylamino)ethyl)-1H-indol-4-ol dihydrogen phosphate ester
3-2'-Dimethylaminoethylindol-4-phosphate
O-Phosphoryl-4-hydroxy-N,N-dimethyltryptamine
4-Phosphoryloxy-N,N-dimethyltryptamine
Psilocibin
Psilocin phosphate ester
Psilotsibin
Teonanacatl
Psylocybin

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: QVDSEJDULKLHCG-UHFFFAOYSA-N
Formula: C12H17N2O4P
SMILES: CN(C)CCc1c[nH]c2cccc(OP(=O)(O)O)c12
Mol. weight [g/mol]: 284.25
CAS: 520-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	1.262		Crippen Method
mccvol	204.920	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=C520525&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/24-313-7/Psilocybine.pdf>

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