

Psilocin

Other names:

1H-Indol-4-ol, 3-[2-(dimethylamino)ethyl]-
Indol-4-ol, 3-[2-(dimethylamino)ethyl]-
CX 59
N,N-Dimethyl-4-Hydroxytryptamine
Psilocine
4-Hydroxy-N,N-dimethyltryptamine
3-(2-(Dimethylamino)ethyl)indol-4-ol
Psilotsin

Inchi:

3-[2-(dimethylamino)ethyl]-1H-indol-4-ol

InchiKey:

SPCIYGNTAMCTRO-UHFFFAOYSA-N

Formula:

C₁₂H₁₆N₂O

SMILES:

CN(C)CCc1c[nH]c2ccc(O)c12

Mol. weight [g/mol]:

204.27

CAS:

520-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.496		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpol	1980.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook

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=C520536&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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