

1H-Indole-3-ethanamine, 5-methoxy-

Other names:	1H-Indole-3-ethanamine, 5-methoxy- Indole, 3-(2-aminoethyl)-5-methoxy- Methoxytryptamine 3-(2-Aminoethyl)-5-methoxyindole 5MOT Meksamin (free base) Mexamine Mexamine base Ethanamine,2-(5-methoxy-3-indolyl)- 2-(5-Methoxyindol-3-yl)ethylaniline NSC 56422
Inchi:	InChI=1S/C11H14N2O/c1-14-9-2-3-11-10(6-9)8(4-5-12)7-13-11/h2-3,6-7,13H,4-5,12H2,1
InchiKey:	JTEJPPKMYBDEMY-UHFFFAOYSA-N
Formula:	C11H14N2O
SMILES:	COc1ccc2[nH]cc(CCN)c2c1
Mol. weight [g/mol]:	190.25

Physical Properties

Property code	Value	Unit	Source
ie	7.68 ± 0.12	eV	NIST Webbook
log10ws	-2.74		Cheméo Relay (1.0)
logp	1.196		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
tf	410.08	K	Cheméo Relay (1.0)

Sources

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=C608071&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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