Etryptamine

Other names:	(.+/-.)-Etryptamine
	1H-Indole-3-ethanamine, «alpha»-ethyl-
	1H-Indole-3-ethanamine, Â«alphaÂ»-ethyl-
	3-(2-Aminobutyl)indole
	3-Indolylbutylamine
	Ethyltryptamine
	Indole, 3-(2-aminobutyl)-
	NSC 88061
	Ro 3-1932
	«alpha»-Ethyltryptamine
	Â«alphaÂ»-Ethyltryptamine
Inchi:	InChI=1S/C12H16N2/c1-2-10(13)7-9-8-14-12-6-4-3-5-11(9)12/h3-6,8,10,14H,2,7,13H2,1
InchiKey:	ZXUMUPVQYAFTLF-UHFFFAOYSA-N
Formula:	C12H16N2
SMILES:	CCC(N)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	188.27
CAS:	2235-90-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Aqueous Solubility Prediction Method
logp	1.966		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
rinpol	1848.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2235907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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