Indole, 3-(2-(diethylamino)ethyl)-

Other names:	D.E.T. N,N-Diethyltryptamine Diethyltryptamine
Inchi:	InChI=1S/C14H20N2/c1-3-16(4-2)10-9-12-11-15-14-8-6-5-7-13(12)14/h5-8,11,15H,3-4,9-
InchiKey:	LSSUMOWDTKZHHT-UHFFFAOYSA-N
Formula:	C14H20N2
SMILES:	CCN(CC)CCc1c[nH]c2ccccc12
Mol. weight [g/mol]:	216.32
CAS:	61-51-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	2.570		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
rinpol	1875.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1875.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C61518&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices