

Desmethylclozapine

Other names:	N-Desmethylclozapine
Inchi:	InChI=1S/C17H17ClN4/c18-12-5-6-15-16(11-12)21-17(22-9-7-19-8-10-22)13-3-1-2-4-14
InchiKey:	JNNOSTQEZICQQP-UHFFFAOYSA-N
Formula:	C17H17ClN4
SMILES:	<chem>Clc1ccc2c(c1)N=C(N1CCNCC1)c1ccccc1N2</chem>
Mol. weight [g/mol]:	312.80
CAS:	6104-71-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	3.380		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
rinsol	3001.40		NIST Webbook
rinsol	3001.40		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6104718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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