

Uniconazole-p, trimethylsilyl ether

Other names:	Uniconazole, tms derivative
Inchi:	InChI=1S/C18H26ClN3OSi/c1-18(2,3)17(23-24(4,5)6)16(22-13-20-12-21-22)11-14-7-9-10
InchiKey:	OOQHGEFLJITJJM-WJDWOHSUSA-N
Formula:	C18H26ClN3OSi
SMILES:	CC(C)(C)C(O[Si](C)(C)C)C(=Cc1ccc(Cl)cc1)n1cncn1
Mol. weight [g/mol]:	363.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	5.196		Crippen Method
rinpol	2245.90		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U334057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/120-717-2/Uniconazole-p-trimethylsilyl-ether.pdf>

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