

Pregabalin, N-trimethylsilyl-, trimethylsilyl ester

Inchi:	InChI=1S/C14H33NO2Si2/c1-12(2)9-13(11-15-18(3,4)5)10-14(16)17-19(6,7)8/h12-13,15
InchiKey:	YRQMVHPCJPTUJU-UHFFFAOYSA-N
Formula:	C14H33NO2Si2
SMILES:	CC(C)CC(CN[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	303.59

Physical Properties

Property code	Value	Unit	Source
log10ws	0.65		Crippen Method
logp	3.841		Crippen Method
rinpol	1494.80		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U417172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/124-376-7/Pregabalin-N-trimethylsilyl-trimethylsilyl-ester.pdf>

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