

Milnacipran, N-trimethylsilyl-

Inchi: InChI=1S/C18H30N2OSi/c1-6-20(7-2)17(21)18(15-11-9-8-10-12-15)13-16(18)14-19-22(3)
InchiKey: WBHQJVSTXQUMNA-UHFFFAOYSA-N
Formula: C18H30N2OSi
SMILES: CCN(CC)C(=O)C1(c2ccccc2)CC1CN[Si](C)(C)C
Mol. weight [g/mol]: 318.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	3.237		Crippen Method
rinpol	2031.30		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417205&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/99-371-1/Milnacipran-N-trimethylsilyl.pdf>

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