Desmethyldoxepin, N-trimethylsilyl-

Inchi: InChI=1S/C21H27NOSi/c1-22(24(2,3)4)15-9-13-19-18-11-6-5-10-17(18)16-23-21-14-8-7-
InchiKey: FSKYDGSNDYHCAJ-UYRXBGFRSA-N
Formula: C21H27NOSi
SMILES: CN(CCC=C1c2ccccc2COc2ccccc21)[Si](C)(C)C
Mol. weight [g/mol]: 337.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	5.167		Crippen Method
rinpol	2424.60		NIST Webbook
rinpol	2424.60		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U417185&Units=SI

Legend

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