

Venlafaxine, trimethylsilyl ether

Inchi: InChI=1S/C20H35NO2Si/c1-21(2)16-19(17-10-12-18(22-3)13-11-17)20(23-24(4,5)6)14-8
InchiKey: ZUCFIIIQBQECIW-UHFFFAOYSA-N
Formula: C20H35NO2Si
SMILES: COc1ccc(C(CN(C)C)C2(O[Si](C)(C)C)CCCC2)cc1
Mol. weight [g/mol]: 349.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	4.895		Crippen Method
rinpol	2100.10		NIST Webbook
rinpol	2100.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417235&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/121-918-8/Venlafaxine-trimethylsilyl-ether.pdf>

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