

Alprenolol, N-trimethylsilyl-, trimethylsilyl ether

Other names:	Alprenolol, 2tms derivative
Inchi:	InChI=1S/C21H39NO2Si2/c1-10-13-19-14-11-12-15-21(19)23-17-20(24-26(7,8)9)16-22(10)20
InchiKey:	XUNRRDCXXWUGPE-UHFFFAOYSA-N
Formula:	C ₂₁ H ₃₉ NO ₂ Si ₂
SMILES:	<chem>C=CCc1cccc1OCC(CN(C(C)C)[Si](C)(C)C)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	393.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	5.559		Crippen Method
rinsol	2070.40		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333827&Units=SI

Legend

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

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