

Bisoprolol, TBDMS

Inchi: InChI=1S/C24H45NO4Si/c1-19(2)25-16-23(29-30(8,9)24(5,6)7)18-28-22-12-10-21(11-13)
InchiKey: MIUUVROBIQDCOS-UHFFFAOYSA-N
Formula: C24H45NO4Si
SMILES: CC(C)NCC(COC1ccc(COCCOC(C)C)cc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 439.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	5.395		Crippen Method
rinpol	2591.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417465&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/125-211-8/Bisoprolol-TBDMS.pdf>

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