

Atenolol, TBDMS

Inchi: InChI=1S/C26H50N2O3Si2/c1-20(2)28-18-23(30-32(9,10)25(3,4)5)19-29-22-15-13-21(14)
InchiKey: WSZVSLUSPKHZAO-UHFFFAOYSA-N
Formula: C26H50N2O3Si2
SMILES: CC(C)NCC(COc1ccc(CC(=N)O[Si](C)(C)C(C)(C)C)cc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 494.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	6.995		Crippen Method
rinsol	2857.50		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435140&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/66-687-7/Atenolol-TBDMS.pdf>

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