

Timolol, PFB-TMS

Inchi: InChI=1S/C20H31F7N4O4SSi/c1-17(2,3)31(16(32)18(21,22)19(23,24)20(25,26)27)11-13
InchiKey: JLNXCXADSXSCRfZ-UHFFFAOYSA-N
Formula: C20H31F7N4O4SSi
SMILES: CC(C)(C)N(CC(COc1nsnc1N1CCOCC1)O[Si](C)(C)C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 584.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	4.434		Crippen Method
rinpol	2853.00		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=R175061&Units=SI>

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/80-548-5/Timolol-PFB-TMS.pdf>

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