

Alprenolol, tert-butyldimethylsilyl ether

Other names: Alprenolol, TBDMS
Alprenolol, tbdms derivative

Inchi: InChI=1S/C21H37NO2Si/c1-9-12-18-13-10-11-14-20(18)23-16-19(15-22-17(2)3)24-25(7,
InchiKey: VRQHRSXIGWWRJE-UHFFFAOYSA-N

Formula: C₂₁H₃₇NO₂Si

SMILES: C=CCc1cccc1OCC(CNC(C)C)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 363.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	5.182		Crippen Method
rinpol	2069.70		NIST Webbook
rinpol	2084.10		NIST Webbook
rinpol	2069.70		NIST Webbook
rinpol	2084.10		NIST Webbook

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=U333829&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/94-675-9/Alprenolol-tert-butyldimethylsilyl-ether.pdf>

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