

Isoprenaline, N-TFA-O-TMS

Inchi: InChI=1S/C22H40F3NO4Si3/c1-16(2)26(21(27)22(23,24)25)15-20(30-33(9,10)11)17-12-
InchiKey: WYVLXNFPHPNSER-UHFFFAOYSA-N
Formula: C22H40F3NO4Si3
SMILES: CC(C)N(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)C(F)(F)F
Mol. weight [g/mol]: 523.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.36		Crippen Method
logp	6.806		Crippen Method
rinpol	2056.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R208423&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/77-419-2/Isoprenaline-N-TFA-O-TMS.pdf>

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