

p-Synephrine, DTFMB-TMS

Other names:	p-Synephrine, N-DTFMB-TMS
Inchi:	InChI=1S/C24H31F6NO3Si2/c1-31(22(32)17-12-18(23(25,26)27)14-19(13-17)24(28,29)3
InchiKey:	FTLDSFURVGIGJP-UHFFFAOYSA-N
Formula:	C24H31F6NO3Si2
SMILES:	CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)cc1)C(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	551.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	7.603		Crippen Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		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=R54214&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/119-845-2/p-Synephrine-DTFMB-TMS.pdf>

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