Adrenaline, N-DTFMB-TMS

Other names:	Adrenaline, DTFMB-TMS
Inchi:	InChI=1S/C27H39F6NO4Si3/c1-34(25(35)19-13-20(26(28,29)30)16-21(14-19)27(31,32)3
InchiKey:	PGCARAXUUGXVRZ-UHFFFAOYSA-N
Formula:	C27H39F6NO4Si3
SMILES:	CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)c1cc(C(F)(F)F)cc(C(F
Mol. weight [g/mol]:	639.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	8.816		Crippen Method
rinpol	2386.00		NIST Webbook
rinpol	2386.00		NIST Webbook
rinpol	2386.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164942&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/58-792-9/Adrenaline-N-DTFMB-TMS.pdf
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