

(-)-Bunolol, PFB-TMS

Inchi:	InChI=1S/C27H32F5NO4Si/c1-27(2,3)33(26(35)20-21(28)23(30)25(32)24(31)22(20)29)1
InchiKey:	DZGLEEKVLFHXAV-UHFFFAOYSA-N
Formula:	C27H32F5NO4Si
SMILES:	CC(C)(C)N(CC(CO)c1cccc2c1CCCC2=O)O[Si](C)(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	557.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	6.441		Crippen Method
rinpol	2961.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R175016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/54-422-3/Bunolol-PFB-TMS.pdf>

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