

Benzeneethanamine, N-[(pentafluorophenyl)methylene]-«beta»,4-bis[(tr

Other names:	Octopamine, PFB-imine, TMS
Inchi:	InChI=1S/C21H26F5NO2Si2/c1-30(2,3)28-14-9-7-13(8-10-14)16(29-31(4,5)6)12-27-11-1
InchiKey:	LKJPSAODMMZLQD-UHFFFAOYSA-N
Formula:	C21H26F5NO2Si2
SMILES:	C[Si](C)(C)Oc1ccc(C(CN=Cc2c(F)c(F)c(F)c(F)c2F)O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	475.60
CAS:	55429-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	6.607		Crippen Method
rinpola	2159.00		NIST Webbook
rinpola	2159.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55429851&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
rinpola:	Non-polar retention indices

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