

# Benzeneethanamine, N-[(pentafluorophenyl)methylene]-4-[(trimethylsilyl)

Other names:	Tyramine, PFB-imine, TMS
Inchi:	InChI=1S/C18H18F5NOSi/c1-26(2,3)25-12-6-4-11(5-7-12)8-9-24-10-13-14(19)16(21)18(
InchiKey:	RQUNKHLYXVYWVK-UHFFFAOYSA-N
Formula:	C18H18F5NOSi
SMILES:	C[Si](C)(C)Oc1ccc(CCN=Cc2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]:	387.42
CAS:	55334-64-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	5.257		Crippen Method
rinpola	2012.00		NIST Webbook
rinpola	2012.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334640&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

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