

# Benzeneethanamine, N-[(pentafluorophenyl)methylene]-«beta»-[(trimethylsilyloxy)ethyl]ammonium

Other names:	2-Hydroxy-2-phenylethylamine, PFB-imine, TMS
Inchi:	InChI=1S/C18H18F5NOSi/c1-26(2,3)25-13(11-7-5-4-6-8-11)10-24-9-12-14(19)16(21)18(20)22
InchiKey:	OCLLTNUKNVMOOC-UHFFFAOYSA-N
Formula:	C18H18F5NOSi
SMILES:	C[Si](C)(C)OC(CN=Cc1c(F)c(F)c(F)c(F)c1F)c1ccccc1
Mol. weight [g/mol]:	387.42
CAS:	55334-63-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	5.394		Crippen Method
rinpola	1859.00		NIST Webbook
rinpola	1859.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334639&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334639&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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