

# Benzeneethanamine, 4-methoxy-N-[(pentafluorophenyl)methylene]-3-[(t

Other names:	2-(3-Hydroxy-4-methoxyphenyl)ethylamine, PFB-imine, TMS
Inchi:	InChI=1S/C19H20F5NO2Si/c1-26-13-6-5-11(9-14(13)27-28(2,3)4)7-8-25-10-12-15(20)17
InchiKey:	XSRGUHNJXDKJOO-UHFFFAOYSA-N
Formula:	C19H20F5NO2Si
SMILES:	COc1ccc(CCN=Cc2c(F)c(F)c(F)c(F)c2F)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	417.45
CAS:	55556-73-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	5.266		Crippen Method
rinpol	2127.00		NIST Webbook
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## Sources

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=C55556735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55556735&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>

## Legend

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

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