3,4-Dimethoxyphenylthylamine, N-trimethylsilyl-

Other names: Benzeneethanamine, 3,4-dimethoxy, mono-TMS
3,4-Dimethoxyphenethylamine, tms derivative

Inchi: InChI=1S/C13H23NO2Si/c1-15-12-7-6-11(10-13(12)16-2)8-9-14-17(3,4)5/h6-7,10,14H,8-

InchiKey: XTOHFXVDOGRZMG-UHFFFAOYSA-N

Formula: C13H23NO2Si

SMILES: COc1ccc(CCN[Si](C)(C)C)cc1OC

Mol. weight [g/mol]: 253.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	2.671		Crippen Method
rinpol	1721.50		NIST Webbook
rinpol	1721.50		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333952&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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