4-Bromo-2,5-dimethoxyphenethylamine, N-trimethylsilyl-

Inchi: InChI=1S/C13H22BrNO2Si/c1-16-12-9-11(14)13(17-2)8-10(12)6-7-15-18(3,4)5/h8-9,15H

InchiKey: LTSMHXBNVXWRNH-UHFFFAOYSA-N

Formula: C13H22BrNO2Si

SMILES: COc1cc(CCN[Si](C)(C)C)c(OC)cc1Br

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	3.433		Crippen Method
rinpol	1949.90		NIST Webbook
rinpol	1949.90		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U417181&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices