Benzeneacetic acid, 3,4-dimethoxy-, trimethylsilyl ester

Other names: Acetic acid, (3,4-dimethoxyphenyl)-, trimethylsilyl ester
Homoveratric acid, TMS
Homoveratric acid, tms derivative

Inchi: InChI=1S/C13H20O4Si/c1-15-11-7-6-10(8-12(11)16-2)9-13(14)17-18(3,4)5/h6-8H,9H2,1-

InchiKey: ZOTLJAZLFPDMSU-UHFFFAOYSA-N

Formula: C13H20O4Si

SMILES: COc1ccc(CC(=O)O[Si](C)(C)C)cc1OC

Mol. weight [g/mol]: 268.38

CAS: 27750-60-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	2.624		Crippen Method
rinpol	1726.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1682.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750603&Units=SI

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

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

Legend

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