

# Benzenepropanoic acid, 3-methoxy-«alpha»,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Benzenepropanoic acid, «alpha»,4-dihydroxy-3-methoxy, tris-TMS

Inchi: InChI=1S/C19H36O5Si3/c1-21-17-13-15(11-12-16(17)22-25(2,3)4)14-18(23-26(5,6)7)19

InchiKey: AXGULIYEKPVHPG-UHFFFAOYSA-N

Formula: C19H36O5Si3

SMILES: COc1cc(CC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 428.74

CAS: 55887-61-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.50		Crippen Method
logp	5.050		Crippen Method
rinpol	2028.00		NIST Webbook
rinpol	2022.00		NIST Webbook
rinpol	2028.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887611&Units=SI>

## Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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