Mandelic acid, 3-hydroxy-4-methoxy, TMS

Inchi: InChI=1S/C18H34O5Si3/c1-20-15-12-11-14(13-16(15)21-24(2,3)4)17(22-25(5,6)7)18(19)
InchiKey: RSMKYYXMOYFGLI-UHFFFAOYSA-N
Formula: C18H34O5Si3
SMILES: COc1ccc(C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 414.72

Physical Properties

Property code	Value	Unit	Source
log10ws	1.58		Crippen Method
logp	5.180		Crippen Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R95032&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