

Benzeneacetic acid, 4-methoxy-«alpha»-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names

p-Methoxymandelic acid (2TMS)

Mandelic acid, 4-methoxy, bis-TMS

Mandelic acid, 4-methoxy, TMS

4-Methoxymandelic acid, 2tms derivative

Inchi:	InChI=1S/C15H26O4Si2/c1-17-13-10-8-12(9-11-13)14(18-20(2,3)4)15(16)19-21(5,6)7/h8
InchiKey:	YPMJZCBYIBICBB-UHFFFAOYSA-N
Formula:	C15H26O4Si2
SMILES:	COc1ccc(C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	326.54
CAS:	55556-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.58		Crippen Method
logp	3.966		Crippen Method
rinpol	1697.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55556951&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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