

Benzeneacetic acid, 3-methoxy-«alpha»-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names

M-methoxymandelic acid (2TMS)

Mandelic acid, 3-methoxy, bis-TMS

Mandelic acid, 3-methoxy, TMS

M-methoxymandelic acid, 2tms derivative

Inchi:	InChI=1S/C15H26O4Si2/c1-17-13-10-8-9-12(11-13)14(18-20(2,3)4)15(16)19-21(5,6)7/h8
InchiKey:	WGEAHMOFUVPHPD-UHFFFAOYSA-N
Formula:	C15H26O4Si2
SMILES:	COc1cccc(C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]:	326.54
CAS:	55530-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.58		Crippen Method
logp	3.966		Crippen Method
rinpol	1660.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/30-761-3/Benzeneacetic-acid-3-methoxy-alpha-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

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