

Benzeneacetic acid, 2-methoxy-«alpha»-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: o-Methoxymandelic acid, trimethylsiloxy-, trimethylsilyl ester
o-Methoxymandelic acid (2TMS)

Mandelic acid, 2-methoxy, bis-TMS

Mandelic acid, 2-methoxy, TMS

O-methoxymandelic acid, 2tms derivative

Inchi: InChI=1S/C15H26O4Si2/c1-17-13-11-9-8-10-12(13)14(18-20(2,3)4)15(16)19-21(5,6)7/h8

InchiKey: AXAHAFRCRQFTMF-UHFFFAOYSA-N

Formula: C15H26O4Si2

SMILES: COc1ccccc1C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 326.54

CAS: 55530-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.58		Crippen Method
logp	3.966		Crippen Method
rinsol	1618.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530660&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

rinsol: Non-polar retention indices

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