

# Benzeneacetic acid, «alpha»,4-bis[(tert-butyl dimethylsilyl)oxy]-3-methoxy- tert-butyl dimethylsilyl ester

Other names:	DL-4-hydroxy-3-methoxymandelic acid, bis(tert-butyl dimethylsilyl) ether, tert-Butyl(dimethyl)silyl ether, tert-Butyl(dimethyl)silyl pyrrol[tert-butyl(dimethyl)silyl]oxymorpho(4-pyrrol[tert-butyl(dimethyl)silyl]oxymorpho-3-methoxy-4-hydroxy-3-methoxy-1-phenylethanoate, Vanillylmandelic acid, tert-BDMS Vanillylmandelic acid, TBDMS Vanillylmandelic acid, 3tdbms derivative
Inchi:	InChI=1S/C27H52O5Si3/c1-25(2,3)33(11,12)30-21-18-17-20(19-22(21)29-10)23(31-34(1
InchiKey:	CGCMIBHFTPWWNW-UHFFFAOYSA-N
Formula:	C27H52O5Si3
SMILES:	COc1cc(C(O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	540.96
CAS:	78324-20-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	8.691		Crippen Method
rinpol	2511.00		NIST Webbook
rinpol	2481.40		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2481.40		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2511.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324206&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324206&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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