

4-Hydroxymandelic acid, tris(O-t-butyl dimethylsilyl)-

Other names:	p-Hydroxymandelic acid, TBDMS p-Hydroxymandelic acid, DMTBS 4-Hydroxymandelic acid, 3tdms derivative
Inchi:	InChI=1S/C26H50O4Si3/c1-24(2,3)31(10,11)28-21-18-16-20(17-19-21)22(29-32(12,13)2
InchiKey:	DNJVKPPMOZUSN-UHFFFAOYSA-N
Formula:	C26H50O4Si3
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]:	510.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	8.682		Crippen Method
rinsol	2423.00		NIST Webbook
rinsol	2427.00		NIST Webbook
rinsol	2400.00		NIST Webbook

Sources

Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U71882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemo.com/cid/13-153-7/4-Hydroxymandelic-acid-tris-O-t-butyl dimethylsilyl.pdf>

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