Mandelic acid di(tert-butyldimethylsilyl)-

Other names:	Benzeneacetic acid, «alpha»-[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester DL-Mandelic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester Mandelic acid, bis-TBDMS Mandelic acid, TBDMS Mandelic acid, DMTBS tert-Butyl(dimethyl)silyl ([tert-butyl(dimethyl)silyl]oxy)(phenyl)acetate Mandelic acid, 2tbdms derivative
Inchi:	InChI=1S/C20H36O3Si2/c1-19(2,3)24(7,8)22-17(16-14-12-11-13-15-16)18(21)23-25(9,10
InchiKey:	FNVJWYFVHSEHFW-UHFFFAOYSA-N
Formula:	C20H36O3Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C(O[Si](C)(C)C(C)(C)C)c1ccccc1
Mol. weight [g/mol]:	380.67
CAS:	78324-07-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	6.298		Crippen Method
rinpol	1886.20		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1886.20		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324079&Units=SI

Legend

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