Benzeneacetic acid, «alpha»,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Mandelic acid, 4-hydroxy, tris-TMS
	Mandelic acid, 4-hydroxy, (3TMS)-
	Mandelic acid, 4-hydroxy, TMS
	Mandelic acid, 4-hydroxy, bis-TMS
	4-Hydroxymandelic acid, 3tms derivative
Inchi:	InChI=1S/C17H32O4Si3/c1-22(2,3)19-15-12-10-14(11-13-15)16(20-23(4,5)6)17(18)21-24
InchiKey:	YPRXSYQBVBCYJZ-UHFFFAOYSA-N
Formula:	C17H32O4Si3
SMILES:	C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	384.69
CAS:	37148-64-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.70		Crippen Method
logp	5.171		Crippen Method
rinpol	1782.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1790.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37148644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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