Benzeneacetic acid, «alpha»,3,4-tris[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	3,4-Dihydroxymandelic acid, (tetrakis-TMS)-
	Trimethylsilyl 3,4-dihydroxymandelate tris(trimethylsilyl) ether
	Trimethylsilyl (3,4-bis[(trimethylsilyl)oxy]phenyl)[(trimethylsilyl)oxy]acetate
	Mandelic acid, 3,4-dihydroxy, tetrakis-TMS
	Mandelic acid, 3,4-dihydroxy, (4TMS)-
	Mandelic acid, 3,4-dihydroxy, TMS
	3,4-Dihydroxymandelic acid, 4tms derivative
Inchi:	InChI=1S/C20H40O5Si4/c1-26(2,3)22-17-14-13-16(15-18(17)23-27(4,5)6)19(24-28(7,8)9
InchiKey:	MDAKQGIALDYWHV-UHFFFAOYSA-N
Formula:	C20H40O5Si4
SMILES:	C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	472.87
CAS:	37148-65-5

Physical Properties

Property code	Value	Unit	Source
log10ws	2.69		Crippen Method
logp	6.385		Crippen Method
rinpol	1938.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1938.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37148655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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