Benzeneacetic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Othernames:	3,4-Dihydroxyphenylacetic acid (tms)
	Trimethylsilyl (3,4-bis[(trimethylsilyl)oxy]phenyl)acetate
	Benzeneacetic acid, 3,4-dihydroxy, tris-TMS
	Homoprotocatechuic acid, tris-TMS
	Phenylacetic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester
	Phenylacetic acid, 3,4-dihydroxy, (3TMS)-
	Benzeneacetic acid, 3,4-dihydroxy, TMS
	Homoprotocatechuic acid, TMS
	Phenylacetic acid, 3,4-dihydroxy, TMS
	3,4-Dihydroxyphenylacetic acid, 3tms derivative
Inchi:	InChI=1S/C17H32O4Si3/c1-22(2,3)19-15-11-10-14(12-16(15)20-23(4,5)6)13-17(18)21-24
InchiKey:	RYYDTJQPEUISHG-UHFFFAOYSA-N
Formula:	C17H32O4Si3
SMILES:	C[Si](C)(C)OC(=O)Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	384.69
CAS:	37148-62-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.54		Crippen Method
logp	5.035		Crippen Method
rinpol	1833.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1827.60		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1827.60		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=C37148622&Units=SI

Legend

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