

3-(3-Hydroxyphenyl)-3-hydroxypropionic acid, tris-(O-trimethylsilyl)-

Other names:	m-Trimethylsilyloxyphenyl(trimethylsilyloxy)trimethylsilylacrylate 3-(3-Hydroxyphenyl)hydracrylic acid, tri-TMS 3-(3-Hydroxy-phenyl)-3-hydroxypropionic acid, triTMS
Inchi:	InChI=1S/C18H34O4Si3/c1-23(2,3)20-16-12-10-11-15(13-16)17(21-24(4,5)6)14-18(19)2
InchiKey:	UXEHNGHKNIKDF-UHFFFAOYSA-N
Formula:	C18H34O4Si3
SMILES:	C[Si](C)(C)OC(=O)CC(O[Si](C)(C)C)c1cccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	398.72

Physical Properties

Property code	Value	Unit	Source
log10ws	1.28		Crippen Method
logp	5.561		Crippen Method
rmpol	1864.00		NIST Webbook
rmpol	1867.00		NIST Webbook
rmpol	1870.00		NIST Webbook
rmpol	1869.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U71697&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
rmpol:	Non-polar retention indices

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