Glycine, N-(trimethylsilyl)-N-[2-[(trimethylsilyl)oxy]benzoyl trimethylsilyl ester

Other names:	2-Hydroxyhippuric acid, N,O,O-tris(trimethylsilyl) deriv.
	2-Hydroxyhippuric acid, tris-TMS
	2-Hydroxyhippuric acid, 3tms derivative
Inchi:	InChI=1S/C18H33NO4Si3/c1-24(2,3)19(14-17(20)23-26(7,8)9)18(21)15-12-10-11-13-16(
InchiKey:	SJLWAPOSGSUWJU-UHFFFAOYSA-N
Formula:	C18H33NO4Si3
SMILES:	C[Si](C)(C)OC(=O)CN(C(=O)c1ccccc1O[Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]:	411.72
CAS:	55517-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.90		Crippen Method
logp	4.556		Crippen Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1954.00		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=C55517538&Units=SI

Legend

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

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https://www.chemeo.com/cid/56-737-2/Glycine-N-trimethylsilyl-N-2-trimethylsilyl-oxy-benzoyl-trimethylsilyl-ester.pdf

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