Hippuric acid, 3-hydroxy, TMS, # 1

Inchi:	InChI=1S/C18H33NO4Si3/c1-24(2,3)21-16-12-10-11-15(13-16)18(23-26(7,8)9)19-14-17(
InchiKey:	DMQDEQYREHGSLU-HNENSFHCSA-N
Formula:	C18H33NO4Si3
SMILES:	C[Si](C)(C)OC(=O)CN=C(O[Si](C)(C)C)c1cccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	411.72

Physical Properties

Property code	Value	Unit	Source
log10ws	1.97		Crippen Method
logp	4.877		Crippen Method
rinpol	2055.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R94674&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

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