Syringic acid (2TMS)

Inchi:	InChI=1S/C15H26O5Si2/c1-17-12-9-11(15(16)20-22(6,7)8)10-13(18-2)14(12)19-21(3,4)5
InchiKey:	KWOFGVXBWXVAJU-UHFFFAOYSA-N
Formula:	C15H26O5Si2
SMILES:	COc1cc(C(=O)O[Si](C)(C)C)cc(OC)c1O[Si](C)(C)C
Mol. weight [g/mol]:	342.53

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	3.909		Crippen Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		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=U413963&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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