Protocatechuic aldehyde, TMS

Inchi:	InChI=1S/C13H22O3Si2/c1-17(2,3)15-12-8-7-11(10-14)9-13(12)16-18(4,5)6/h7-10H,1-6H
InchiKey:	SUXBXVBGVLEZAU-UHFFFAOYSA-N
Formula:	C13H22O3Si2
SMILES:	C[Si](C)(C)Oc1ccc(C=O)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	282.48

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	3.926		Crippen Method
rinpol	1618.00		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=R403128&Units=SI

Legend

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

Latest version available from:

https://www.chemeo.com/cid/34-084-1/Protocatechuic-aldehyde-TMS.pdf

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