4-Hydroxybenzoic acid, 2tbdms derivative

Inchi:	InChI=1S/C19H34O3Si2/c1-18(2,3)23(7,8)21-16-13-11-15(12-14-16)17(20)22-24(9,10)19
InchiKey:	NZUMUAWQJATSIJ-UHFFFAOYSA-N
Formula:	C19H34O3Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]:	366.64
CAS:	78324-14-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	6.233		Crippen Method
rinpol	2115.50		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2119.15		NIST Webbook
rinpol	2122.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2115.50		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=C78324148&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/20-008-0/4-Hydroxybenzoic-acid-2tbdms-derivative.pdf

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