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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324148&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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