4-Hydroxybenzoic acid, 2tms derivative

Inchi: InChI=1S/C13H22O3Si2/c1-17(2,3)15-12-9-7-11(8-10-12)13(14)16-18(4,5)6/h7-10H,1-6H
InchiKey: XVCXIVAVMFNKDH-UHFFFAOYSA-N
Formula: C13H22O3Si2
SMILES: C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 282.48
CAS: 2078-13-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	3.892		Crippen Method
rinpol	1620.50		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1628.60		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1620.50		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1628.60		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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