Acetophenone, 4-hydroxy-3-methoxy, oxime, bis-TMS

Inchi: InChI=1S/C15H27NO3Si2/c1-12(16-19-21(6,7)8)13-9-10-14(15(11-13)17-2)18-20(3,4)5/h

InchiKey: CUHGNLCZOBUSCD-VBKFSLOCSA-N

Formula: C15H27NO3Si2

SMILES: COc1cc(C(C)=NO[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 325.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.05		Crippen Method
logp	4.484		Crippen Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R99937&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

Latest version available from:

https://www.chemeo.com/cid/42-244-4/Acetophenone-4-hydroxy-3-methoxy-oxime-bis-TMS.pdf

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