

2-Nonenoic acid, 4-hydroxy, TMS, methyl ester, # 2

Inchi: InChI=1S/C13H26O3Si/c1-6-7-8-9-12(16-17(3,4)5)10-11-13(14)15-2/h10-12H,6-9H2,1-5H3
InchiKey: ZMPSQEQNDMMHLY-UHFFFAOYSA-N
Formula: C13H26O3Si
SMILES: CCCCCC(C=CC(=O)OC)O[Si](C)(C)C
Mol. weight [g/mol]: 258.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Crippen Method
logp	3.516		Crippen Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398902&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/124-628-7/2-Nonenoic-acid-4-hydroxy-TMS-methyl-ester-2.pdf>

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