

(E)-10-Dodecenoic acid, 9-hydroxy-12-oxo, methyl ester, MSTFA adduct, OH-TMS, # 2

Inchi: InChI=1S/C22H42F3NO5Si2/c1-26(21(28)22(23,24)25)19(31-33(6,7)8)17-16-18(30-32(3
InchiKey: JEUZFGKDQQMND E-WUKNDPDISA-N
Formula: C22H42F3NO5Si2
SMILES: COC(=O)CCCCCCC(C=CC(O[Si](C)(C)C)N(C)C(=O)C(F)(F)F)O[Si](C)(C)C
Mol. weight [g/mol]: 513.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	5.865		Crippen Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554939&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/59-769-4/E-10-Dodecenoic-acid-9-hydroxy-12-oxo-methyl-ester-MSTFA-adduct-OH-TM>

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