

(E)-10-Dodecenoic acid, 9-hydroxy-12-oxo, methyl ester, PFB-oxime, OH-TMS, # 1

Inchi: InChI=1S/C23H32F5NO4Si/c1-31-18(30)13-9-7-5-6-8-11-16(33-34(2,3)4)12-10-14-29-32
InchiKey: KMAJTMRPYQAYKG-OAVGYLGISA-N
Formula: C23H32F5NO4Si
SMILES: COC(=O)CCCCCCC(C=CC=NOCc1c(F)c(F)c(F)c(F)c1F)O[Si](C)(C)C
Mol. weight [g/mol]: 509.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.91		Crippen Method
logp	6.564		Crippen Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		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=R554944&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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