(E)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, «omega»-PFB-oxime, TMS-enol, # 1

Inchi: InChI=1S/C23H30F5NO4Si/c1-31-18(30)13-9-7-5-6-8-11-16(33-34(2,3)4)12-10-14-29-32

InchiKey: JSJKNWKLXHWHPR-XIBWGEAYSA-N

Formula: C23H30F5NO4Si

SMILES: COC(=O)CCCCCCC=C(C=CC=NOCc1c(F)c(F)c(F)c(F)c1F)O[Si](C)(C)C

Mol. weight [g/mol]: 507.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	6.690		Crippen Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R554895&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