

(Z)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, «omega»-PFB-oxime, TMS-enol, # 2

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-QBAYRTSVSA-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
logp	6.690		Crippen Method
rinpol	2679.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554999&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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