

GA7 di-acid 9,10-ene, methyl ester TMS ether

Inchi: InChI=1S/C23H32O4Si/c1-14-12-23-13-15(14)9-10-17(23)16-8-7-11-22(2,21(25)27-28(4
InchiKey: XIMSJWRVAKBHJV-KTKRRTNUSA-N
Formula: C23H32O4Si
SMILES: C=C1CC23CC1CCC2=C1C=CCC(C)(C(=O)O[Si](C)(C)C)C1C3C(=O)OC
Mol. weight [g/mol]: 400.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	4.793		Crippen Method
rinpol	2405.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R191018&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/30-807-2/GA7-di-acid-9-10-ene-methyl-ester-TMS-ether.pdf>

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