

GA20-15-ene, Me-TMS

Inchi: InChI=1S/C23H34O5Si/c1-14-12-21-13-22(14,28-29(4,5)6)11-8-15(21)23-10-7-9-20(2,19)
InchiKey: LQQPMSFHYIQPQS-HHBZDXFNSA-N
Formula: C23H34O5Si
SMILES: COC(=O)C1C2C3(C)CCCC2(OC3=O)C2CCC3(O[Si](C)(C)C)CC12C=C3C
Mol. weight [g/mol]: 418.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	4.228		Crippen Method
rinpol	2432.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R547496&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/57-232-1/GA20-15-ene-Me-TMS.pdf>

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