

[14C] GA31 methyl ester TMS ether

Inchi: InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)15(28-29(4,5)6)10-16(22)23-9-7-8-21(2,20)
InchiKey: YTEJWGMOWVRFPN-XBIMHJGDSA-N
Formula: C₂₃H₃₂O₅Si
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	3.860		Crippen Method
rinpol	2546.00		NIST Webbook
rinpol	2557.00		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=R190882&Units=SI>

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/66-849-7/14C-GA31-methyl-ester-TMS-ether.pdf>

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