

[13C]GA5 methyl ester TMS ether

Other names:	[14C] GA5 methyl ester TMS ether
Inchi:	InChI=1S/C23H32O5Si/c1-14-12-21-13-22(14,28-29(4,5)6)11-8-15(21)23-10-7-9-20(2,19)
InchiKey:	JKQCNZHRNGPPQX-HHBZDXFNSA-N
Formula:	C23H32O5Si
SMILES:	C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]:	416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.004		Crippen Method
rinpol	2475.00		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2475.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R181581&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/28-373-7/13C-GA5-methyl-ester-TMS-ether.pdf>

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