

[13C]GA8 methyl ester TMS ether

Other names:	[2H2]GA8, MeTMS
Inchi:	InChI=1S/C29H50O7Si3/c1-18-15-27-17-28(18,36-39(10,11)12)14-13-20(27)29-16-19(34)
InchiKey:	URXALWQXBINWJP-QKOPFLJYSA-N
Formula:	C29H50O7Si3
SMILES:	C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)(C(=O)O)O1
Mol. weight [g/mol]:	594.96

Physical Properties

Property code	Value	Unit	Source
log10ws	0.33		Crippen Method
logp	5.888		Crippen Method
rinpol	2816.00		NIST Webbook
rinpol	2845.00		NIST Webbook
rinpol	2843.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R178699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/40-000-6/13C-GA8-methyl-ester-TMS-ether.pdf>

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