

GA39, methyl ester TMS

Other names:	GA39, MeTMS
Inchi:	InChI=1S/C29H48O8Si2/c1-17-15-28-16-18(17)19(36-38(6,7)8)14-20(28)29(26(32)35-5)
InchiKey:	SLGPATXYODBIAO-YOCQBWLGSA-N
Formula:	C29H48O8Si2
SMILES:	C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)OC)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1
Mol. weight [g/mol]:	580.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	4.951		Crippen Method
rinpol	2776.00		NIST Webbook
rinpol	2769.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R79515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/67-737-0/GA39-methyl-ester-TMS.pdf>

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