

GA7-diacid, methyl ester TMS ether

Other names:	iso-GA7 open lactone, MeTMS
Inchi:	InChI=1S/C27H44O6Si2/c1-17-15-26-16-18(17)11-12-19(26)27(33-35(8,9)10)14-13-20(3
InchiKey:	ORTXOSLRHLEBAW-QGPPGHEHSA-N
Formula:	C27H44O6Si2
SMILES:	C=C1CC23CC1CCC2C1(O[Si](C)(C)C)C=CC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)C
Mol. weight [g/mol]:	520.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	5.327		Crippen Method
rinpola	2573.00		NIST Webbook
rinpola	2575.00		NIST Webbook
rinpola	2573.00		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=R181383&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-356-6/GA7-diacid-methyl-ester-TMS-ether.pdf>

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