

GA2, Me-TMS

Other names:	GA2 methyl ester TMS ether GA2, MeTMSi
Inchi:	InChI=1S/C26H44O6Si2/c1-23(32-34(7,8)9)15-25-14-16(23)10-11-17(25)26-13-12-18(31)
InchiKey:	UNSOQWMOWIREFY-WGYAJBHMSA-N
Formula:	C26H44O6Si2
SMILES:	<chem>COC(=O)C1C2C3(CCC(O[Si](C)(C)C)C2(C)C(=O)O3)C2CCC3CC12CC3(C)O[Si](C)(C)O</chem>
Mol. weight [g/mol]:	508.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	5.138		Crippen Method
rinpol	2761.00		NIST Webbook
rinpol	2762.00		NIST Webbook
rinpol	2745.00		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=R79412&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/40-871-0/GA2-Me-TMS.pdf>

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