

GA13, MeTMS

Other names:	GA13 methyl ester TMS ether GA13, methyl ester TMS
Inchi:	InChI=1S/C26H40O7Si/c1-15-13-25-14-16(15)9-10-17(25)26(23(29)32-5)12-11-18(33-34)
InchiKey:	KCLVZLRNSUVMTD-LNNHUYSYSA-N
Formula:	C26H40O7Si
SMILES:	<chem>C=C1CC23CC1CCC2C1(C(=O)OC)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)OC</chem>
Mol. weight [g/mol]:	492.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	4.121		Crippen Method
rinpol	2567.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2586.00		NIST Webbook
rinpol	2592.00		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2597.00		NIST Webbook
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
rinpol	2596.00		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=R79216&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.cheméo.com/cid/38-565-3/GA13-MeTMS.pdf>

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