

GA127 methyl ester TMS ether

Inchi:	InChI=1S/C28H48O6Si2/c1-18-16-27-17-28(18,34-36(9,10)11)20(33-35(6,7)8)15-19(27)2
InchiKey:	KASWOOFZNVOGAL-ASNICIOVSA-N
Formula:	C28H48O6Si2
SMILES:	C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C1(C)CCCC(C)(C(=O)OC)C1C3C(=O
Mol. weight [g/mol]:	536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	5.942		Crippen Method
rinpol	2662.00		NIST Webbook
rinpol	2663.00		NIST Webbook
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R334666&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.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.chemeo.com/cid/28-639-2/GA127-methyl-ester-TMS-ether.pdf>

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