

GA38, methyl ester TMS

Other names: GA38, MeTMS
Inchi: InChI=1S/C27H44O6Si2/c1-17-14-26-15-27(17,33-35(7,8)9)13-10-18(26)25-12-11-19(32)
InchiKey: FGHFCLKJWQGLGR-JUCSEYGPISA-N
Formula: C27H44O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CCC(O[Si](C)(C)C)C(C)(C(=O)OC1)C2C3C(=O)C3
Mol. weight [g/mol]: 520.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Crippen Method
logp	5.306		Crippen Method
rinpol	2940.00		NIST Webbook
rinpol	2988.00		NIST Webbook
rinpol	2989.00		NIST Webbook
rinpol	2940.00		NIST Webbook
rinpol	2961.00		NIST Webbook
rinpol	2988.00		NIST Webbook
rinpol	2961.00		NIST Webbook
rinpol	2991.00		NIST Webbook
rinpol	2939.00		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=R79501&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/21-688-5/GA38-methyl-ester-TMS.pdf>

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