

[13C]GA29 methyl ester TMS ether

Other names: [2H2]GA29, MeTMS
Inchi: InChI=1S/C26H42O6Si2/c1-16-12-24-15-25(16,32-34(7,8)9)11-10-18(24)26-14-17(31-33)23-22-21-20-19-18
InchiKey: AINOJINHWCGRJ-WGTPPGOWSA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC(O[Si](C)(C)C)CC(C)(C(=O)O1)C2C3C(=O)O1
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	5.058		Crippen Method
rinpol	2682.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2688.00		NIST Webbook
rinpol	2688.00		NIST Webbook
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2682.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178684&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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