

GA58 methyl ester TMS ether

Other names: GA58, MeTMSi
GA58, methyl ester TMS

Inchi: InChI=1S/C26H42O6Si2/c1-15-13-25-14-16(15)17(31-33(4,5)6)12-18(25)26-11-10-19(32

InchiKey: YJIAMACEKPLATL-SGFUFJRXSA-N

Formula: C26H42O6Si2

SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)C

Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	4.914		Crippen Method
rinpol	2742.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2744.00		NIST Webbook
rinpol	2752.00		NIST Webbook
rinpol	2744.00		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=R79725&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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