

GA49 methyl ester TMS ether

Other names: GA49, MeTMSi
GA49, MeTMS
GA49, methyl ester TMS

Inchi: InChI=1S/C29H50O7Si3/c1-17-14-28-15-18(17)19(34-37(4,5)6)13-21(28)29-16-20(35-38)

InchiKey: ZPNFPFWLCLGXCS-GBAHORNQSA-N

Formula: C₂₉H₅₀O₇Si₃

SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)(C(=O)O)O1

Mol. weight [g/mol]: 594.96

Physical Properties

Property code	Value	Unit	Source
log10ws	0.57		Crippen Method
logp	5.744		Crippen Method
rinpol	2837.00		NIST Webbook
rinpol	2831.00		NIST Webbook
rinpol	2836.00		NIST Webbook
rinpol	2844.00		NIST Webbook
rinpol	2836.00		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=R79622&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/56-058-6/GA49-methyl-ester-TMS-ether.pdf>

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