

GA48 methyl ester TMS ether

Other names: GA48, MeTMSi
GA48, MeTMS
GA48, 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-PNLLDYGDSA-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	2796.00		NIST Webbook
rinpol	2787.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2796.00		NIST Webbook
rinpol	2805.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79618&Units=SI>

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

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.cheméo.com/cid/17-272-1/GA48-methyl-ester-TMS-ether.pdf>

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