

OH GA12-like, methyl ester TMS ether

Other names: [2H2]GA53, MeTMS
Inchi: InChI=1S/C25H40O5Si/c1-16-14-24-15-25(16,30-31(6,7)8)13-10-17(24)22(2)11-9-12-23
InchiKey: TVWDMRKJNXNYSE-SCDURKMASA-N
Formula: C₂₅H₄₀O₅Si
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C1(C)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 448.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	5.112		Crippen Method
rinpole	2556.00		NIST Webbook
rinpole	2588.00		NIST Webbook
rinpole	2584.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R204590&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/55-314-2/OH-GA12-like-methyl-ester-TMS-ether.pdf>

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