

GA36 MeTMS

Other names: GA36 methyl ester TMS ether
Inchi: InChI=1S/C25H38O6Si/c1-15-12-25-13-16(15)8-9-17(25)24(14-26)11-10-18(31-32(5,6)7
InchiKey: ZHPKKVOJDKMYED-HOXWFPEYSA-N
Formula: C₂₅H₃₈O₆Si
SMILES: C=C1CC23CC1CCC2C1(C=O)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 462.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	4.146		Crippen Method
rinpol	2582.00		NIST Webbook
rinpol	2578.00		NIST Webbook
rinpol	2584.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2600.00		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=R79480&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/15-180-5/GA36-MeTMS.pdf>

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