

GA114, MeTMS

Inchi: InChI=1S/C24H36O5Si/c1-14-11-24-12-15(14)10-16(29-30(4,5)6)18(24)23-9-7-8-22(2,21)
InchiKey: DEFMWDBHSXPSNB-OIEVWUHNSA-N
Formula: C24H36O5Si
SMILES: C=C1CC23CC1CC(O[Si](C)(C)C)C2C12CCCC(C)(C(=O)OC1)C2C3C(=O)OC
Mol. weight [g/mol]: 432.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	4.331		Crippen Method
rinpol	2915.00		NIST Webbook
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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=R270894&Units=SI>

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.chemeo.com/cid/61-340-6/GA114-MeTMS.pdf>

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