

GA115, MeTMS

Inchi: InChI=1S/C25H38O6Si/c1-15-12-25-13-16(15)11-17(31-32(5,6)7)19(25)24(14-26)10-8-9
InchiKey: FHZACGVEEDSLHN-FZMUJSPDSA-N
Formula: C25H38O6Si
SMILES: C=C1CC23CC1CC(O[Si](C)(C)C)C2C1(C=O)CCCC(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	2708.00		NIST Webbook
rinpol	2709.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270903&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.chemeo.com/cid/46-218-9/GA115-MeTMS.pdf>

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