

GA39 3-isovalerate, methyl ester TMS

Inchi: InChI=1S/C31H48O9Si/c1-17(2)13-23(32)39-22-11-12-31(28(35)38-7)21-14-20(40-41(8),
InchiKey: JNZAETUXJDJJTN-RKDJDSNISA-N
Formula: C31H48O9Si
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)OC)CCC(OC(=O)CC(C)C)C(C)(C(=O)OC)
Mol. weight [g/mol]: 592.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	4.688		Crippen Method
rinpol	3067.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258790&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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/29-405-0/GA39-3-isovalerate-methyl-ester-TMS.pdf>

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