

GA64, MeTMS

Inchi: InChI=1S/C24H36O5Si/c1-14-15-8-9-16-23-11-7-10-22(2,21(26)28-13-23)18(23)17(20(21)24)12-3-5-6-4-2
InchiKey: MCCYRDQWTJLJCQ-KLVLLYGESA-N
Formula: C₂₄H₃₆O₅Si
SMILES: C=C1C2CCC3C45CCCC(C)(C(=O)OC4)C5C(C(=O)OC)C3(C2)C1O[Si](C)(C)C
Mol. weight [g/mol]: 432.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	4.331		Crippen Method
rinpol	2754.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79793&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/24-660-2/GA64-MeTMS.pdf>

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