

GA14, MeTMS

Inchi: InChI=1S/C25H40O5Si/c1-15-13-25-14-16(15)9-10-17(25)23(2)12-11-18(30-31(6,7)8)24
InchiKey: QQEYOHKHRLMQMP-ZGHKCMSCSA-N
Formula: C25H40O5Si
SMILES: C=C1CC23CC1CCC2C1(C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 448.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	4.967		Crippen Method
rinpol	2497.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2496.00		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2506.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79220&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/35-246-0/GA14-MeTMS.pdf>

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