

GA27, MeTMS

Inchi: InChI=1S/C27H44O6Si2/c1-16-12-26-13-17(16)10-11-19(26)27-14-18(32-34(4,5)6)22(33)
InchiKey: IUFJAUNUNQPFBX-YSJORRDESA-N
Formula: C27H44O6Si2
SMILES: C=C1CC23CC1CCC2C12COC(=O)C(C)(C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1)C2C3C(=O)
Mol. weight [g/mol]: 520.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.99		Crippen Method
logp	5.161		Crippen Method
rinpol	2865.00		NIST Webbook
rinpol	2861.00		NIST Webbook
rinpol	2897.00		NIST Webbook
rinpol	2865.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79373&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/41-776-5/GA27-MeTMS.pdf>

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