

3-epi GA54, MeTMSi

Inchi: InChI=1S/C26H42O6Si2/c1-15-13-25-14-16(15)10-11-17(25)26-19(32-34(7,8)9)12-18(31)
InchiKey: GIRWPRDLMDKQLW-SKNAWRDLA-N
Formula: C₂₆H₄₂O₆Si₂
SMILES: C=C1CC23CC1CCC2C12OC(=O)C(C)(C(O[Si](C)(C)C)CC1O[Si](C)(C)C)C2C3C(=O)OC
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	4.914		Crippen Method
rinpol	2638.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258478&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/61-160-6/3-epi-GA54-MeTMSi.pdf>

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