

PGA1, methyl ester, trimethylsilyl ether

Other names: 3-epi-GA1, MeTMS
Inchi: InChI=1S/C24H42O4Si/c1-6-7-10-13-21(28-29(3,4)5)18-16-20-17-19-23(25)22(20)14-11
InchiKey: LEEKIWQCOFKZII-FBMGVBCBSA-N
Formula: C24H42O4Si
SMILES: CCCCCC(C=CC1C=CC(=O)C1CCCCCCC(=O)OC)O[Si](C)(C)C
Mol. weight [g/mol]: 422.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	6.228		Crippen Method
rinpola	2802.00		NIST Webbook
rinpola	2788.00		NIST Webbook
rinpola	2788.00		NIST Webbook
rinpola	2796.00		NIST Webbook
rinpola	2788.00		NIST Webbook
rinpola	2782.00		NIST Webbook
rinpola	2781.00		NIST Webbook
rinpola	2802.00		NIST Webbook
rinpola	2782.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368687&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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