

11-«alpha»-Hydroxy-9,15-cyclo-GA9, methyl ester [D2], TMS

Inchi: InChI=1S/C23H32O5Si/c1-12-13-10-14(28-29(4,5)6)23-16(12)21(23,11-13)15(18(24)26-3
InchiKey: HMLNHQYKESBMFJ-ZMNXUOQGSA-N
Formula: C23H32O5Si
SMILES: C=C1C2CC(O[Si](C)(C)C)C34C1C3(C2)C(C(=O)OC)C1C2(C)CCCC14OC2=O
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	3.694		Crippen Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499753&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/99-221-7/11-alpha-Hydroxy-9-15-cyclo-GA9-methyl-ester-D2-TMS.pdf>

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