

GA121 (1,2-didehydro GA70), MeTMS

Inchi: InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)15(28-29(4,5)6)10-16(22)23-9-7-8-21(2,20)
InchiKey: GGKPYEWCDNJRKB-XBIMHJG YSA-N
Formula: C23H32O5Si
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12C=CCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	3.860		Crippen Method
rinsol	2561.00		NIST Webbook
rinsol	2563.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R281151&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-695-4/GA121-1-2-didehydro-GA70-MeTMS.pdf>

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