

GA122-isolactone, 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-BMDCNDRESA-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
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R281077&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/16-114-7/GA122-isolactone-MeTMS.pdf>

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