

# GA95-isolactone, MeTMS

**Inchi:** InChI=1S/C23H32O5Si/c1-14-12-21-13-22(14,28-29(4,5)6)11-8-15(21)23-10-7-9-20(2,19)  
**InchiKey:** CWTLMASHPLNKBZ-YBMAXVMDSA-N  
**Formula:** C23H32O5Si  
**SMILES:** C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=CCC(C)(C(=O)O1)C2C3C(=O)OC  
**Mol. weight [g/mol]:** 416.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.004		Crippen Method
rinpol	2600.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2600.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270849&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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<https://www.chemeo.com/cid/35-216-3/GA95-isolactone-MeTMS.pdf>

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