

ent-7-Hydroxy kaurenoic acid, MeTMSi

Other names:	ent-Kaurenoic acid, 7-hydroxy, methyl ester, TMS
Inchi:	InChI=1S/C24H40O3Si/c1-16-14-24-15-17(16)9-10-18(24)22(2)11-8-12-23(3,21(25)26-4
InchiKey:	YXFQNPBASJUBAH-PTRFMDCRSA-N
Formula:	C24H40O3Si
SMILES:	C=C1CC23CC1CCC2C1(C)CCCC(C)(C(=O)OC)C1CC3O[Si](C)(C)C
Mol. weight [g/mol]:	404.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	5.958		Crippen Method
rinpola	2367.00		NIST Webbook
rinpola	2367.00		NIST Webbook
rinpola	2367.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R79113&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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/36-620-3/ent-7-Hydroxy-kaurenoic-acid-MeTMSi.pdf>

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