

7-Oxodehydroabietic acid, trimethylsilyl ester

Other names:	7-Oxo-dehydroabietic acid TMS ester
Inchi:	InChI=1S/C23H34O3Si/c1-15(2)16-9-10-18-17(13-16)19(24)14-20-22(18,3)11-8-12-23(2)
InchiKey:	WDUYGEDKWUTMKQ-UHFFFAOYSA-N
Formula:	C23H34O3Si
SMILES:	<chem>CC(C)c1ccc2c(c1)C(=O)CC1C(C)(C(=O)O[Si](C)(C)C)CCCC21C</chem>
Mol. weight [g/mol]:	386.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	5.839		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292793&Units=SI

Legend

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

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