Dehydroabietic acid, trimethylsilyl ester

Other names:	Dehydroabietic acid, TMS
	Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, trimethylsilyl ester
	Abieta-8,11,13-trienoic acid, TMS ester
	Dehydroabietic acid TMS ester
	Dehydroabietic acid, tms derivative
Inchi:	InChI=1S/C23H36O2Si/c1-16(2)17-9-11-19-18(15-17)10-12-20-22(19,3)13-8-14-23(20,4)
InchiKey:	HSHYFFAXUHETAU-UHFFFAOYSA-N
Formula:	C23H36O2Si
SMILES:	CC(C)c1ccc2c(c1)CCC1C(C)(C(=O)O[Si](C)(C)C)CCCC21C
Mol. weight [g/mol]:	372.62
CAS:	21414-49-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	6.198		Crippen Method
rinpol	2385.00		NIST Webbook
rinpol	2373.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21414493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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