ABIETIC ACID, TRIMETHYLSILYL ESTER

Other names:	Podocarpa-7,13-dien-15-oic acid, 13-isopropyl-, trimethylsilyl ester
	Abietic acid (TMS)
	Abietic acid TMS ester
	Abietic acid, tms derivative
Inchi:	InChI=1S/C23H38O2Si/c1-16(2)17-9-11-19-18(15-17)10-12-20-22(19,3)13-8-14-23(20,4)
InchiKey:	RXWFRYPIQODUHW-UHFFFAOYSA-N
Formula:	C23H38O2Si
SMILES:	CC(C)C1=CC2=CCC3C(C)(C(=O)O[Si](C)(C)C)CCCC3(C)C2CC1
Mol. weight [g/mol]:	374.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Cheméo Relay (1.0)
logp	6.500		Crippen Method
rinpol	2422.70		NIST Webbook
rinpol	2412.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2412.00		NIST Webbook
rinpol	2422.70		NIST Webbook
tf	371.21	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21414506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point