

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:	RXWFRYP IQODUHW-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]:	374.63
CAS:	21414-50-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	6.500		Crippen Method
rinpol	2412.00		NIST Webbook
rinpol	2422.70		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21414506&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/99-203-7/Abietic-acid-trimethylsilyl-ester.pdf>

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