DEHYDROABIETIC ACID, TRIMETHYLSILYL ESTER

Other names: Abieta-8,11,13-trienoic acid, TMS ester
Dehydroabietic acid TMS ester
Dehydroabietic acid, TMS
Dehydroabietic acid, tms derivative
Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, trimethylsilyl ester

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

Physical Properties

Property code	Value	Unit	Source
logp	6.198		Crippen Method
tf	352.10	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

tf: Normal melting (fusion) point