7,15-Dihydroxydehydroabietic acid, tris(trimethylsilyl)deriv.

Other names: 7,15-Dihydroxydehydroabietic acid, tri-TMS
Inchi: InChI=1S/C29H52O4Si3/c1-27(2,33-36(11,12)13)21-15-16-23-22(19-21)24(31-34(5,6)7)2
InchiKey: VVDBQEDXBMVTKV-UHFFFAOYSA-N
Formula: C29H52O4Si3
SMILES: CC(C)(O[Si](C)(C)C)c1ccc2c(c1)C(O[Si](C)(C)C)CC1C(C)(C(=O)O[Si](C)(C)C)CCCC21C
Mol. weight [g/mol]: 548.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	8.512		Crippen Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292803&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