(-)-11-nor-9-carboxy-.DELTA.9-THC, trimethylsilyl ether, trimethylsilyl ester

Inchi: InChI=1S/C27H44O4Si2/c1-10-11-12-13-19-16-23-25(24(17-19)30-32(4,5)6)21-18-20(26

InchiKey: RLALMBCUXILXIS-UHFFFAOYSA-N

Formula: C27H44O4Si2

SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C)c1)C1C=C(C(=O)O[Si](C)(C)C)CCC1C(C)(C)O2

Mol. weight [g/mol]: 488.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	7.602		Crippen Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U417170&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