.beta.-isovaleryl echinatine, diTMS

Inchi: InChI=1S/C26H49NO6Si2/c1-18(2)16-23(28)31-20(5)26(19(3)4,33-35(9,10)11)25(29)30-
InchiKey: SXBAWEVBZGPMEF-XDDOSOJWSA-N
Formula: C26H49NO6Si2
SMILES: CC(C)CC(=O)O[C@@H](C)[C@](O[Si](C)(C)C)(C(=O)OCC1=CCN2CC[C@H](O[Si](C)(C)
Mol. weight [g/mol]: 527.85

Physical Properties

Property code	Value	Unit	Source
logp	4.988		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R252336
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