«beta»-tiglyl-trachelanthamine, TMS

Inchi: InChI=1S/C23H41NO5Si/c1-9-17(4)21(25)28-18(5)23(16(2)3,29-30(6,7)8)22(26)27-15-19
InchiKey: HMRJKPOSMZQFJQ-WSBWIDHSSA-N
Formula: C23H41NO5Si
SMILES: CC=C(C)C(=O)OC(C)C(O[Si](C)(C)C)(C(=O)OCC1CCN2CCCC12)C(C)C
Mol. weight [g/mol]: 439.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	4.158		Crippen Method
rinpol	2475.00		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=R252356&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices