Benzoylecgonine, tert-butyldimethylsilyl ester

Other names: Benzoylecgonine, tbdms derivative
Inchi: InChI=1S/C22H33NO4Si/c1-22(2,3)28(5,6)27-21(25)19-17-13-12-16(23(17)4)14-18(19)2
InchiKey: ABCVHKZYHPKTKB-UHFFFAOYSA-N
Formula: C22H33NO4Si
SMILES: CN1C2CCC1C(C(=O)O[Si](C)(C)C(C)(C)C)C(OC(=O)c1ccccc1)C2
Mol. weight [g/mol]: 403.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	4.243		Crippen Method
rinpol	2569.70		NIST Webbook
rinpol	2569.70		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352939&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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