

Benzoylnorecgonine, tert-butyldimethylsilyl ester

Inchi:	InChI=1S/C21H31NO4Si/c1-21(2,3)27(4,5)26-20(24)18-16-12-11-15(22-16)13-17(18)25-
InchiKey:	ZFHDHHGAFAAQMX-UHFFFAOYSA-N
Formula:	C21H31NO4Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C1C2CCC(CC1OC(=O)c1ccccc1)N2
Mol. weight [g/mol]:	389.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	3.901		Crippen Method
rinpol	2547.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/59-650-5/Benzoylnorecgonine-tert-butyldimethylsilyl-ester.pdf>

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