

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)c1cccc1)C2
Mol. weight [g/mol]:	403.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	4.243		Crippen Method
rinsol	2569.70		NIST Webbook
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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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/113-317-4/Benzoylecgonine-tert-butyldimethylsilyl-ester.pdf>

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