

# Benzoylecgonine, tert-butyldimethylsilyl ester

<b>Other names:</b>	Benzoylecgonine, tbdms derivative
<b>Inchi:</b>	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
<b>InchiKey:</b>	ABCVHKZYHPKTKB-UHFFFAOYSA-N
<b>Formula:</b>	C22H33NO4Si
<b>SMILES:</b>	CN1C2CCC1C(C(=O)O[Si](C)(C)C(C)(C)C)C(OC(=O)c1cccc1)C2
<b>Mol. weight [g/mol]:</b>	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

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

## Legend

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

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

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