

# Benzoylecgonine-TMS

<b>Other names:</b>	Benzoylecgonine, o-trimethylsilyl- Benzoylecgonine, trimethylsilyl ester
<b>Inchi:</b>	InChI=1S/C19H27NO4Si/c1-20-14-10-11-15(20)17(19(22)24-25(2,3)4)16(12-14)23-18(2
<b>InchiKey:</b>	XJVQJFLZKCKXME-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO4Si
<b>SMILES:</b>	CN1C2CCC1C(C(=O)O[Si](C)(C)C)C(OC(=O)c1ccccc1)C2
<b>Mol. weight [g/mol]:</b>	361.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	3.073		Crippen Method
rinpol	2323.20		NIST Webbook
rinpol	2323.20		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U352940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352940&amp;Units=SI</a>

## Legend

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

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