

# 1,3-Dimethylthiopental

<b>Other names:</b>	Thiopentone, permethylated Thiopental permethylated
<b>Inchi:</b>	InChI=1S/C13H22N2O2S/c1-6-8-9(3)13(7-2)10(16)14(4)12(18)15(5)11(13)17/h9H,6-8H2
<b>InchiKey:</b>	DZSBVSFFHQBTFT-UHFFFAOYSA-N
<b>Formula:</b>	C13H22N2O2S
<b>SMILES:</b>	CCCC(C)C1(CC)C(=O)N(C)C(=S)N(C)C1=O
<b>Mol. weight [g/mol]:</b>	270.39
<b>CAS:</b>	80783-03-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	2.034		Crippen Method
mcvol	218.320	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C80783035&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C80783035&amp;Units=SI</a>
<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>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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