

# Thiopental Me, #2

**Inchi:** InChI=1S/C13H22N2O2S/c1-6-8-9(3)13(7-2)10(16)14-12(18-5)15(4)11(13)17/h9H,6-8H2  
**InchiKey:** MFZQGQHIKISKPH-UHFFFAOYSA-N  
**Formula:** C13H22N2O2S  
**SMILES:** CCCC(C)C1(CC)C(=O)N=C(SC)N(C)C1=O  
**Mol. weight [g/mol]:** 270.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.537		Crippen Method
mcvol	218.320	ml/mol	McGowan Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R40603&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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