

# Secobarbital, 1,3-dibutyl

**Other names:** Secobarbital perbutylated  
**Inchi:** InChI=1S/C21H36N2O3/c1-6-10-13-17(5)21(14-9-4)18(24)22(15-11-7-2)20(26)23(19(21)  
**InchiKey:** FMRLVZYGTGAVCZ-UHFFFAOYSA-N  
**Formula:** C21H36N2O3  
**SMILES:** C=CCC1(C(C)CCCC)C(=O)N(CCCC)C(=O)N(CCCC)C1=O  
**Mol. weight [g/mol]:** 364.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	4.766		Crippen Method
mcvol	316.260	ml/mol	McGowan Method
rinpol	2052.00		NIST Webbook
rinpol	2056.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2060.00		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=R387645&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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