Allobarbital perbutylated

Inchi: InChI=1S/C18H28N2O3/c1-5-9-13-19-15(21)18(11-7-3,12-8-4)16(22)20(17(19)23)14-10-

InchiKey: KDKNPSYYGLUITQ-UHFFFAOYSA-N

Formula: C18H28N2O3

SMILES: C=CCC1(CC=C)C(=O)N(CCCC)C(=O)N(CCCC)C1=O

Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.516		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1894.00		NIST Webbook

Sources

Crippen Method: 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=R387709&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