

Barbital perbutylated

Inchi: InChI=1S/C16H28N2O3/c1-5-9-11-17-13(19)16(7-3,8-4)14(20)18(15(17)21)12-10-6-2/h5
InchiKey: LWQHYRGKDABXIQ-UHFFFAOYSA-N
Formula: C16H28N2O3
SMILES: CCCCNC(=O)N(CCCC)C(=O)C(CC)(CC)C1=O
Mol. weight [g/mol]: 296.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	3.184		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
rinpole	1840.00		NIST Webbook
rinpole	1840.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R387729&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/48-418-5/Barbital-perbutylated.pdf>

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