

Hexobarbital perbutylated

Inchi: InChI=1S/C16H24N2O3/c1-4-5-11-18-14(20)16(2,12-9-7-6-8-10-12)13(19)17(3)15(18)21
InchiKey: FHGBKAGAEGHTAM-UHFFFAOYSA-N
Formula: C16H24N2O3
SMILES: CCCCNC(=O)N(C)C(=O)C(C)(C2=CCCCC2)C1=O
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.714		Crippen Method
mcvol	234.950	ml/mol	McGowan Method
rinpola	2042.00		NIST Webbook
rinpola	2042.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R387912&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-331-9/Hexobarbital-perbutylated.pdf>

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