

Metharbital perbutylated

Inchi: InChI=1S/C13H22N2O3/c1-5-8-9-15-11(17)13(6-2,7-3)10(16)14(4)12(15)18/h5-9H2,1-4H
InchiKey: DWNGAZYRZIXVOL-UHFFFAOYSA-N
Formula: C13H22N2O3
SMILES: CCCCN1C(=O)N(C)C(=O)C(CC)(CC)C1=O
Mol. weight [g/mol]: 254.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	2.013		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R387987&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/118-355-7/Metharbital-perbutylated.pdf>

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