Mephobarbital perbutylated

Inchi: InChI=1S/C17H22N2O3/c1-4-6-12-19-15(21)17(5-2,13-10-8-7-9-11-13)14(20)18(3)16(19
InchiKey: CZBRPDNKLQLXFB-UHFFFAOYSA-N
Formula: C17H22N2O3
SMILES: CCCCN1C(=O)N(C)C(=O)C(CC)(c2ccccc2)C1=O
Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.555		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R387967&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:
https://www.chemeo.com/cid/124-479-3/Mephobarbital-perbutylated.pdf
Generated by Cheméo on 2024-04-29 14:29:07.122832453 +0000 UTC m=+16690196.043409768.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.