Amobarbital perbutylated

Inchi: InChI=1S/C19H34N2O3/c1-6-9-13-20-16(22)19(8-3,12-11-15(4)5)17(23)21(18(20)24)14-
InchiKey: ZIZXHFVRSVUKJC-UHFFFAOYSA-N
Formula: C19H34N2O3
SMILES: CCCCN1C(=O)N(CCCC)C(=O)C(CC)(CCC(C)C)C1=O
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	4.210		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1990.00		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=R387714&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