Amobarbital perethylated

Other names: Amobarbital ethylated
Amobarbital, 1,3-diethyl
Inchi: InChI=1S/C15H26N2O3/c1-6-15(10-9-11(4)5)12(18)16(7-2)14(20)17(8-3)13(15)19/h11H
InchiKey: LRKDXQXPQMVDNS-UHFFFAOYSA-N
Formula: C15H26N2O3
SMILES: CCN1C(=O)N(CC)C(=O)C(CC)(CCC(C)C)C1=O
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.650		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1705.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R16068&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices