Pentobarbital ethylated

Other names:	Pentobarbital, 1,3-diethyl
	Pentobarbital perethylated
Inchi:	InChI=1S/C15H26N2O3/c1-6-10-11(5)15(7-2)12(18)16(8-3)14(20)17(9-4)13(15)19/h11H
InchiKey:	SABMZHKJZHPCMB-UHFFFAOYSA-N
Formula:	C15H26N2O3
SMILES:	CCCC(C)C1(CC)C(=O)N(CC)C(=O)N(CC)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	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R16282&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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