Barbital perethylated

Other names: Barbital ethylated
Inchi: InChI=1S/C12H20N2O3/c1-5-12(6-2)9(15)13(7-3)11(17)14(8-4)10(12)16/h5-8H2,1-4H3
InchiKey: KNVYHMMSTFJBMT-UHFFFAOYSA-N
Formula: C12H20N2O3
SMILES: CCN1C(=O)N(CC)C(=O)C(CC)(CC)C1=O
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.623		Crippen Method
mcvol	193.750	ml/mol	McGowan Method
rinpol	1499.00		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=R108388&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

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