Metharbital ethylated

Other names: Metharbital perethylated
Inchi: InChI=1S/C11H18N2O3/c1-5-11(6-2)8(14)12(4)10(16)13(7-3)9(11)15/h5-7H2,1-4H3
InchiKey: WNPZJEMAEJOXCF-UHFFFAOYSA-N
Formula: C11H18N2O3
SMILES: CCN1C(=O)N(C)C(=O)C(CC)(CC)C1=O
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	1.233		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
rinpol	1459.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R108457&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

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