Methylphenobarbital, M(HO-), AC

Inchi: InChI=1S/C15H16N2O5/c1-4-15(12(19)16-14(21)17(3)13(15)20)10-5-7-11(8-6-10)22-9(2
InchiKey: OCXSXUHYEJHCKD-UHFFFAOYSA-N
Formula: C15H16N2O5
SMILES: CCC1(c2ccc(OC(C)=O)cc2)C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 304.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.968		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R255706&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