Methylpseudoecgonine

Inchi: InChI=1S/C17H21NO4/c1-18-12-8-9-14(18)15(13(10-12)17(20)21-2)22-16(19)11-6-4-3-5
InchiKey: YBNSZTYCRZTRRX-FGZQJIAISA-N
Formula: C17H21NO4
SMILES: COC(=O)C1CC2CCC(C1OC(=O)c1ccccc1)N2C
Mol. weight [g/mol]: 303.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.868		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
rinpol	1473.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R510137&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices