Pseudococaine

Other names: [1R-(2-Endo-3-exo)]-3-(benzolyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester
Delcaine
Depsococaine
Dextrocaine
Isococaine

Inchi: InChI=1S/C17H21NO4/c1-18-12-8-9-13(18)15(17(20)21-2)14(10-12)22-16(19)11-6-4-3-5

InchiKey: ZPUCINDJVBIVPJ-YFXXHVASSA-N

Formula: C17H21NO4

SMILES: COC(=O)C1C(OC(=O)c2ccccc2)CC2CCC1N2C

Mol. weight [g/mol]: 303.35

CAS: 478-73-9

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	2180.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C478739&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