Allococaine

Other names:	Methyl 3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate, [1R-(2-exo,3-endo)]- 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, [1R-(2-exo,3-endo)]- (R)-Allococaine Cocaine
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-UHFFFAOYSA-N
Formula:	C17H21NO4
SMILES:	COC(=O)C1C(OC(=O)c2ccccc2)CC2CCC1N2C
Mol. weight [g/mol]:	303.35
CAS:	668-19-9

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C668199&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

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