8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, ethyl ester, [1R-(exo,exo)]-

Other names:	[1R-(Exo,exo)]-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylateacid
	Cocaethylene
	Ethylbenzoylecgonine
	Homocaine
	thylbenzoylecgonine (cocaethylene)
Inchi:	InChI=1S/C18H23NO4/c1-3-22-18(21)16-14-10-9-13(19(14)2)11-15(16)23-17(20)12-7-5-
InchiKey:	NMPOSNRHZIWLLL-UHFFFAOYSA-N
Formula:	C18H23NO4
SMILES:	CCOC(=O)C1C(OC(=O)c2ccccc2)CC2CCC1N2C
Mol. weight [g/mol]:	317.38
CAS:	529-38-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	2.258		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
rinpol	2219.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529384&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