

Pseudococaine

Other names:

[1R-(2-Endo-3-exo)]-3-(benzoyloxy)-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/ci9903071>

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

Latest version available from:

<https://www.cheméo.com/cid/50-106-8/Pseudococaine.pdf>

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