

Benzoylecgonine

Other names:	8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, [1R-(exo,exo)]- 1«alpha»H,5«alpha»H-Tropane-2«beta»-carboxylic acid, 3«beta»-hydroxy-, benzoate, (ester) O-Benzoyl-(-)-ecgonine Ecgonine benzoate Benzoylecgonine 3-(Benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid-, (1R,2R,3S,5S)- O-Benzoylecgonine
Inchi:	InChI=1S/C16H19NO4/c1-17-11-7-8-12(17)14(15(18)19)13(9-11)21-16(20)10-5-3-2-4-6-
InchiKey:	GVGYEFKIHJTNQZ-CLRIEMFWSA-N
Formula:	C16H19NO4
SMILES:	CN1C2CCC1C(C(=O)O)C(OC(=O)c1ccccc1)C2
Mol. weight [g/mol]:	289.33
CAS:	519-09-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	1.779		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
rinpol	2582.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2554.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C519095&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

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