

Formosanan-16-carboxylic acid, 19-methyl-2-oxo-, methyl ester, (19«alpha»)-

Other names:

Mitraphylline
Ajmalicine oxindole B
Mitraphyllin
Rubaradinine
Rubradinin
methyl 19«alpha»-methyl-2-oxoformosanan-16-carboxylate

Inchi: (1'S,3R,4a'S,5a'S,10a'R)-Methyl 1'-methyl-2-oxo-1',4a',5',5a',7',8',10',10a'-octahydrospiro[indoline-3,6'-pyrano[3,4-f]indoliz

InChI=1S/C21H24N2O4/c1:12-14-10-23-8-7-21(16-5-3-4-6-17(16)22-20(21)25)18(23)9-1

InchiKey: JMIAZDVHNCCPDM-UHFFFAOYSA-N

Formula: C21H24N2O4

SMILES: COC(=O)C1=COC(C)C2CN3CCC4(C(=O)Nc5ccccc54)C3CC12

Mol. weight [g/mol]: 368.43

CAS: 509-80-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.062		Crippen Method
mcvol	270.090	ml/mol	McGowan Method
rinpol	3115.30		NIST Webbook
rinpol	3115.30		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C509808&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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