Methyl-12-cytisine acetate

Inchi: InChI=1S/C13H16N2O3/c1-18-13(17)14-6-9-5-10(8-14)11-3-2-4-12(16)15(11)7-9/h2-4,9-
InchiKey: XPJCPQOVGUMVLU-UHFFFAOYSA-N
Formula: C13H16N2O3
SMILES: COC(=O)N1CC2CC(C1)c1cccc(=O)n1C2
Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	1.034		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
rinpol	2176.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R335283&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices