cytisine-12-carboxy-methylester

Inchi: InChI=1S/C13H20N2O3/c1-18-13(17)12-9-5-8(6-14-12)7-15-10(9)3-2-4-11(15)16/h8-10,1
InchiKey: FQQRKEMMBVACFK-UHFFFAOYSA-N
Formula: C13H20N2O3
SMILES: COC(=O)C1NCC2CC1C1CCCC(=O)N1C2
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	0.148		Crippen Method
mcvol	190.420	ml/mol	McGowan Method
rinpol	2240.00		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=R391203&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

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