Hydroxy-N-methylcytisine

Inchi: InChI=1S/C12H16N2O2/c1-13-6-8-5-9(7-13)12(16)14-10(8)3-2-4-11(14)15/h2-4,8-9,12,1
InchiKey: XEYCQYZMQKENBX-UHFFFAOYSA-N
Formula: C12H16N2O2
SMILES: CN1CC2CC(C1)C(O)n1c2cccc1=O
Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	0.388		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
rinpol	2217.00		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=R335263&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