1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, decahydro-3-methyl-

Other names: Cytisine, tetrahydro-12-methyl-
N-methyltetrahydrocytisine

Inchi: InChI=1S/C12H20N2O/c1-13-6-9-5-10(8-13)11-3-2-4-12(15)14(11)7-9/h9-11H,2-8H2,1H

InchiKey: ONDDMIQCYQALKD-UHFFFAOYSA-N

Formula: C12H20N2O

SMILES: CN1CC2CC(C1)C1CCCC(=O)N1C2

Mol. weight [g/mol]: 208.30

CAS: 18161-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	0.949		Crippen Method
mcvol	168.890	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18161950&Units=SI

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

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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