

# 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](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

Latest version available from:

<https://www.cheméo.com/cid/93-714-6/1-5-Methano-8H-pyrido-1-2-a-1-5-diazocin-8-one-decahydro-3-methyl.pdf>

Generated by Cheméo on 2024-04-25 20:59:44.218327482 +0000 UTC m=+16368033.138904793.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.