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

Other names: Cytisine, tetrahydro-
Tetrahydrocytisine

Inchi: InChI=1S/C11H18N2O/c14-11-3-1-2-10-9-4-8(5-12-6-9)7-13(10)11/h8-10,12H,1-7H2

InchiKey: KWVYCGMBGRYVQH-UHFFFAOYSA-N

Formula: C11H18N2O

SMILES: O=C1CCCC2C3CNCC(C3)CN12

Mol. weight [g/mol]: 194.27

CAS: 18161-94-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	0.607		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
rinpol	1843.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1844.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18161949&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