Caulophylline

Other names:	1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-3-methyl-, (1R)- Cytisine, 12-methyl- Caulophyllin N-Methylcytisine 1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-3-methyl-, (1R-cis)- 12-Methylcytisine (1R)-1,2,3,4,5,6-hexahydro-1,5-methano-8H-pyrido[1,2-a][1,5]diazocin-8-one
Inchi:	InChI=1S/C12H16N2O/c1-13-6-9-5-10(8-13)11-3-2-4-12(15)14(11)7-9/h2-4,9-10H,5-8H2
InchiKey:	CULUKMPMGVXCEI-UHFFFAOYSA-N
Formula:	C12H16N2O
SMILES:	CN1CC2CC(C1)c1cccc(=O)n1C2
Mol. weight [g/mol]:	204.27
CAS:	486-86-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	0.897		Crippen Method
mcvol	160.290	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook

Sources

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=C486862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices