

Hydrocotarnine

Other names:	1,3-Dioxolo[4,5-g]isoquinoline, 5,6,7,8-tetrahydro-4-methoxy-6-methyl-Hydrocotarnin 4-Methoxy-6-methyl-5,6,7,8-tetrahydro-1,3-dioxolo(4,5-g)isoquinoline
Inchi:	InChI=1S/C12H15NO3/c1-13-4-3-8-5-10-12(16-7-15-10)11(14-2)9(8)6-13/h5H,3-4,6-7H2
InchiKey:	XXANNZJIZQTCBP-UHFFFAOYSA-N
Formula:	C12H15NO3
SMILES:	COc1c2c(cc3c1OCO3)CCN(C)C2
Mol. weight [g/mol]:	221.25
CAS:	550-10-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.412		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1798.00		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=C550107&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

Latest version available from:

<https://www.cheméo.com/cid/85-535-4/Hydrocotarnine.pdf>

Generated by Cheméo on 2025-12-23 18:13:34.53821634 +0000 UTC m=+6261812.068257003.

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