

1,3-Dioxolo[4,5-g]isoquinolin-5-ol, 5,6,7,8-tetrahydro-6-methyl-

Other names:

Hydraztinine

5,6,7,8-Tetrahydro-6-methyl-1,3-dioxolo(4,5-g)isoquinolin-5-ol

Hydrastinine

Inchi: InChI=1S/C11H13NO3/c1-12-3-2-7-4-9-10(15-6-14-9)5-8(7)11(12)13/h4-5,11,13H,2-3,6H

InchiKey: YOJQZPVUNUQTDF-UHFFFAOYSA-N

Formula: C11H13NO3

SMILES: CN1CCc2cc3c(cc2C1O)OCO3

Mol. weight [g/mol]: 207.23

CAS: 6592-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	0.894		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinsol	1590.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C6592854&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinsol: Non-polar retention indices

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