Dictamnine

Other names:	Furo[2,3-b]quinoline, 4-methoxy- Dictamine Diktaminin
Inchi:	InChI=1S/C12H9NO2/c1-14-11-8-4-2-3-5-10(8)13-12-9(11)6-7-15-12/h2-7H,1H3
InchiKey:	WIONIXOBNMDJFJ-UHFFFAOYSA-N
Formula:	C12H9NO2
SMILES:	COc1c2ccccc2nc2occc12
Mol. weight [g/mol]:	199.21
CAS:	484-29-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.70		Crippen Method
logp	2.990		Crippen Method
mcvol	143.280	ml/mol	McGowan Method
rinpol	1958.10		NIST Webbook
rinpol	1958.10		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=C484297&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

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