

Pteleine

Inchi: InChI=1S/C13H11NO3/c1-15-8-3-4-11-10(7-8)12(16-2)9-5-6-17-13(9)14-11/h3-7H,1-2H3
InchiKey: ALLQMEDAYDKMIO-UHFFFAOYSA-N
Formula: C13H11NO3
SMILES: COc1ccc2nc3occc3c(OC)c2c1
Mol. weight [g/mol]: 229.23
CAS: 2221-41-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	2.998		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
rinpola	2234.10		NIST Webbook
rinpola	2234.10		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2221412&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/116-646-6/Pteleine.pdf>

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