

«gamma»-Fagarine

Inchi: InChI=1S/C13H11NO3/c1-15-10-5-3-4-8-11(10)14-13-9(6-7-17-13)12(8)16-2/h3-7H,1-2H
InchiKey: KFBCTNNQFGONHB-UHFFFAOYSA-N
Formula: C13H11NO3
SMILES: COc1c2ccoc2nc2c(OC)cccc12
Mol. weight [g/mol]: 229.23
CAS: 524-15-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	2.998		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		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=C524152&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/119-013-5/gamma-Fagarine.pdf>

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