

Furo[2,3-b]quinoline, 4,7,8-trimethoxy-

Other names:	«beta»-Fagarine Skimmianin Skimmianine
Inchi:	InChI=1S/C14H13NO4/c1-16-10-5-4-8-11(13(10)18-3)15-14-9(6-7-19-14)12(8)17-2/h4-7
InchiKey:	SLSIBLKBHMKZTB-UHFFFAOYSA-N
Formula:	C14H13NO4
SMILES:	COc1ccc2c(OC)c3ccoc3nc2c1OC
Mol. weight [g/mol]:	259.26
CAS:	83-95-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	3.007		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
rinpol	2375.20		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2375.20		NIST Webbook
rinpol	2330.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83954&Units=SI
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

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/119-579-8/Furo-2-3-b-quinoline-4-7-8-trimethoxy.pdf>

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