

Isoquinoline, 1-methoxy-

Inchi:	InChI=1S/C10H9NO/c1-12-10-9-5-3-2-4-8(9)6-7-11-10/h2-7H,1H3
InchiKey:	AFWHVAFMAIDVTH-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	COc1nccc2ccccc12
Mol. weight [g/mol]:	159.18
CAS:	23724-93-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.243		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

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=C23724938&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/17-672-7/Isoquinoline-1-methoxy.pdf>

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