

Kynurenic acid, methyl ether, methyl ester

Other names:	Methyl 4-methoxyquinoline-2-carboxylate Quinolin-2-carboxylic acid, 4-methoxy, methyl ester
Inchi:	InChI=1S/C12H11NO3/c1-15-11-7-10(12(14)16-2)13-9-6-4-3-5-8(9)11/h3-7H,1-2H3
InchiKey:	BTVCFPOAOCFSJK-UHFFFAOYSA-N
Formula:	C12H11NO3
SMILES:	<chem>COC(=O)c1cc(OC)c2ccccc2n1</chem>
Mol. weight [g/mol]:	217.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.030		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1965.90		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	1965.90		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332748&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
rinpol:	Non-polar retention indices

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