

1-Isoquinolinecarboxylic acid

Other names:	isoquinoline-1-carboxylic acid
Inchi:	InChI=1S/C10H7NO2/c12-10(13)9-8-4-2-1-3-7(8)5-6-11-9/h1-6H,(H,12,13)
InchiKey:	XAAKCCMYRKZRAK-UHFFFAOYSA-N
Formula:	C10H7NO2
SMILES:	O=C(O)c1nccc2ccccc12
Mol. weight [g/mol]:	173.17
CAS:	486-73-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.933		Crippen Method
mcvol	125.960	ml/mol	McGowan Method

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=C486737&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

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