

Methyl 6-chloronicotinate

Other names:	Methyl 2-chloropyridine-5-carboxylate
Inchi:	InChI=1S/C7H6ClNO2/c1-11-7(10)5-2-3-6(8)9-4-5/h2-4H,1H3
InchiKey:	RMEDXVIWDFLGES-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	<chem>COC(=O)c1ccc(Cl)nc1</chem>
Mol. weight [g/mol]:	171.58
CAS:	73781-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.522		Crippen Method
mcvol	115.390	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73781916&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

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