

6-Methylnicotinic acid

Inchi:	InChI=1S/C7H7NO2/c1-5-2-3-6(4-8-5)7(9)10/h2-4H,1H3,(H,9,10)
InchiKey:	RZOKQIPOABEQAM-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Cc1ccc(C(=O)O)cn1
Mol. weight [g/mol]:	137.14
CAS:	3222-47-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.088		Crippen Method
mcvol	103.150	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3222477&Units=SI

Legend

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

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