

6-Methylnicotinamide

Inchi:	InChI=1S/C7H8N2O/c1-5-2-3-6(4-9-5)7(8)10/h2-4H,1H3,(H2,8,10)
InchiKey:	IJXDURUAYOKSIS-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	Cc1ccc(C(N)=O)cn1
Mol. weight [g/mol]:	136.15
CAS:	6960-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	0.489		Crippen Method
mcvol	107.260	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=C6960221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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