2-Carbamoylnicotinic acid

Inchi:	InChI=1S/C7H6N2O3/c8-6(10)5-4(7(11)12)2-1-3-9-5/h1-3H,(H2,8,10)(H,11,12)
InchiKey:	DIABIDLZBNRSPR-UHFFFAOYSA-N
Formula:	C7H6N2O3
SMILES:	NC(=O)c1ncccc1C(=O)O
Mol. weight [g/mol]:	166.13
CAS:	5860-70-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	-0.121		Crippen Method
mcvol	114.700	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=C5860708&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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