

2-Chloro-6-methylpyridine-4-carboxylic acid

Inchi:	InChI=1S/C7H6ClNO2/c1-4-2-5(7(10)11)3-6(8)9-4/h2-3H,1H3,(H,10,11)
InchiKey:	ZGZMEKHQIZSZOH-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	Cc1cc(C(=O)O)cc(Cl)n1
Mol. weight [g/mol]:	171.58
CAS:	25462-85-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	1.742		Crippen Method
mcvol	115.390	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C25462855&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/66-688-6/2-Chloro-6-methylpyridine-4-carboxylic-acid.pdf>

Generated by Cheméo on 2024-04-30 23:40:00.007992715 +0000 UTC m=+16809648.928570042.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.