

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C25462855&Units=SI>
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>

Legend

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

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