

4-Pyridinecarboxylic acid, 2,6-dichloro-

Other names:	Pyridine-4-carboxylic acid, 2,6-dichloro- Pyridine-4-carboxylic acid, 2, 6-dichloro- 2,6-Dichloropyridine-4-carboxylic acid 2,6-dichloroisonicotinic acid
Inchi:	InChI=1S/C6H3Cl2NO2/c7-4-1-3(6(10)11)2-5(8)9-4/h1-2H,(H,10,11)
InchiKey:	SQSYNRCXIZHKAI-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=C(O)c1cc(Cl)nc(Cl)c1
Mol. weight [g/mol]:	192.00
CAS:	5398-44-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	2.087		Crippen Method
mcvol	113.540	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5398447&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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