

2-Thiophenecarboxaldehyde, 5-chloro-

Other names:	5-Chlorothiophene-2-aldehyde 5-Chloro-2-thiophene-carboxaldehyde 5-chlorothiophene-2-carbaldehyde
Inchi:	InChI=1S/C5H3ClOS/c6-5-2-1-4(3-7)8-5/h1-3H
InchiKey:	VWYFITBWBRVBSW-UHFFFAOYSA-N
Formula:	C5H3ClOS
SMILES:	O=Cc1ccc(Cl)s1
Mol. weight [g/mol]:	146.59
CAS:	7283-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	2.214		Crippen Method
mcvol	92.010	ml/mol	McGowan Method

Sources

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=C7283967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/98-440-5/2-Thiophenecarboxaldehyde-5-chloro.pdf>

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