

Ethyl 3,6-dichloropyridine-2-carboxylate

Other names:	2-pyridinecarboxylic acid, 3,6-dichloro-, ethyl ester 3,6-Dichloropyridine-2-carboxylic acid, ethyl ester 3,6-Dichloropicolinic acid, ethyl ester Clopyralid acid, ethyl ester
Inchi:	InChI=1S/C8H7Cl2NO2/c1-2-13-8(12)7-5(9)3-4-6(10)11-7/h3-4H,2H2,1H3
InchiKey:	YWFCLGHVIXWPPZ-UHFFFAOYSA-N
Formula:	C8H7Cl2NO2
SMILES:	CCOC(=O)c1nc(Cl)ccc1Cl
Mol. weight [g/mol]:	220.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	2.565		Crippen Method
mcvol	141.720	ml/mol	McGowan Method
rinpol	1528.00		NIST Webbook

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=U372990&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/10-829-0/Ethyl-3-6-dichloropyridine-2-carboxylate.pdf>

Generated by Cheméo on 2024-04-19 19:08:26.855974973 +0000 UTC m=+15842955.776552285.

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