

Picloram, ethyl ester

Inchi:	InChI=1S/C8H7Cl3N2O2/c1-2-15-8(14)6-3(9)5(12)4(10)7(11)13-6/h2H2,1H3,(H2,12,13)
InchiKey:	NXGNYAVXQNLQRL-UHFFFAOYSA-N
Formula:	C8H7Cl3N2O2
SMILES:	CCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]:	269.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.801		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
rinpole	2577.00		NIST Webbook
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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=U415112&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/119-283-6/Picloram-ethyl-ester.pdf>

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