

Picloram, pentyl ester

Inchi:	InChI=1S/C11H13Cl3N2O2/c1-2-3-4-5-18-11(17)9-6(12)8(15)7(13)10(14)16-9/h2-5H2,1H
InchiKey:	KQYCKQCWZBLLBP-UHFFFAOYSA-N
Formula:	C11H13Cl3N2O2
SMILES:	CCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]:	311.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	3.971		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
rinpole	2895.00		NIST Webbook

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=U415115&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/93-338-4/Picloram-pentyl-ester.pdf>

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