

# Picloram, octyl ester

**Inchi:** InChI=1S/C14H19Cl3N2O2/c1-2-3-4-5-6-7-8-21-14(20)12-9(15)11(18)10(16)13(17)19-12  
**InchiKey:** CYMBTOZDBGCUJT-UHFFFAOYSA-N  
**Formula:** C14H19Cl3N2O2  
**SMILES:** CCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl  
**Mol. weight [g/mol]:** 353.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.10		Crippen Method
logp	5.141		Crippen Method
mcvol	248.480	ml/mol	McGowan Method
rinpole	3220.00		NIST Webbook
rinpole	3220.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415118&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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