

Picloram, hexyl ester

Inchi: InChI=1S/C12H15Cl3N2O2/c1-2-3-4-5-6-19-12(18)10-7(13)9(16)8(14)11(15)17-10/h2-6H
InchiKey: YUSKCJHQDFRFHN-UHFFFAOYSA-N
Formula: C12H15Cl3N2O2
SMILES: CCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 325.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.361		Crippen Method
mcvol	220.300	ml/mol	McGowan Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415116&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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