

Picloram, heptyl ester

Inchi: InChI=1S/C13H17Cl3N2O2/c1-2-3-4-5-6-7-20-13(19)11-8(14)10(17)9(15)12(16)18-11/h2
InchiKey: HPCWHMNQJOAAJN-UHFFFAOYSA-N
Formula: C13H17Cl3N2O2
SMILES: CCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 339.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	4.751		Crippen Method
mcvol	234.390	ml/mol	McGowan Method
rinpole	3109.00		NIST Webbook
rinpole	3109.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415117&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpole: Non-polar retention indices

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