

Picloram, nonyl ester

Inchi: InChI=1S/C15H21Cl3N2O2/c1-2-3-4-5-6-7-8-9-22-15(21)13-10(16)12(19)11(17)14(18)20
InchiKey: LRVNQKKBMWROFC-UHFFFAOYSA-N
Formula: C15H21Cl3N2O2
SMILES: CCCCCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 367.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.531		Crippen Method
mcvol	262.570	ml/mol	McGowan Method
rinpol	3325.00		NIST Webbook
rinpol	3325.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415119&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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

Latest version available from:

<https://www.chemeo.com/cid/78-633-3/Picloram-nonyl-ester.pdf>

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