

Picloram, decyl ester

Inchi: InChI=1S/C16H23Cl3N2O2/c1-2-3-4-5-6-7-8-9-10-23-16(22)14-11(17)13(20)12(18)15(19)
InchiKey: PPCNXZYPHVKAJI-UHFFFAOYSA-N
Formula: C16H23Cl3N2O2
SMILES: CCCCCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 381.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.94		Crippen Method
logp	5.921		Crippen Method
mcvol	276.660	ml/mol	McGowan Method
rinpole	3431.00		NIST Webbook
rinpole	3431.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415120&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

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<https://www.cheméo.com/cid/82-406-0/Picloram-decyl-ester.pdf>

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