

Picloram, heptadecyl ester

Inchi: InChI=1S/C23H37Cl3N2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-30-23(29)21-18
InchiKey: HCCAYVCPGYBWDO-UHFFFAOYSA-N
Formula: C23H37Cl3N2O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 479.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.87		Crippen Method
logp	8.652		Crippen Method
mcvol	375.290	ml/mol	McGowan Method
rinpol	2996.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415127&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/73-735-5/Picloram-heptadecyl-ester.pdf>

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