

Picloram, tetradecyl ester

Inchi: InChI=1S/C20H31Cl3N2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-27-20(26)18-15(21)17(24)
InchiKey: LMZVFVXTYPGIRI-UHFFFAOYSA-N
Formula: C20H31Cl3N2O2
SMILES: CCCCCCCCCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 437.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.61		Crippen Method
logp	7.482		Crippen Method
mcvol	333.020	ml/mol	McGowan Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U415124&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/80-547-6/Picloram-tetradecyl-ester.pdf>

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