Picloram, pentadecyl ester

Inchi:	InChI=1S/C21H33Cl3N2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-28-21(27)19-16(22)18
InchiKey:	DGBABTBBOYLTLJ-UHFFFAOYSA-N
Formula:	C21H33Cl3N2O2
SMILES:	CCCCCCCCCCCCCCCOC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]:	451.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.03		Crippen Method
logp	7.872		Crippen Method
mcvol	347.110	ml/mol	McGowan Method
rinpol	2784.00		NIST Webbook
rinpol	2784.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415125&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

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