

Picloram, isobutyl ester

Inchi: InChI=1S/C10H11Cl3N2O2/c1-4(2)3-17-10(16)8-5(11)7(14)6(12)9(13)15-8/h4H,3H2,1-2H
InchiKey: ZURTZOKKQIXKAL-UHFFFAOYSA-N
Formula: C10H11Cl3N2O2
SMILES: CC(C)COC(=O)c1nc(Cl)c(Cl)c(N)c1Cl
Mol. weight [g/mol]: 297.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Crippen Method
logp	3.437		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
rinpole	2687.00		NIST Webbook
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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=U415113&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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