

Pyraclostrobin

Other names:	Pyraclostrobin Carbamic acid, N-[2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]-N-methoxy-, methyl ester, Carbamic acid, N-[2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]methoxy-, methyl ester methyl [2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]methoxycarbamate
Inchi:	InChI=1S/C19H18ClN3O4/B1-25-19(24)23(26-2)17-6-4-3-5-14(17)13-27-18-11-12-22(21)
InchiKey:	HZRSNVGNWUDEFX-UHFFFAOYSA-N
Formula:	C19H18ClN3O4
SMILES:	<chem>COC(=O)N(OC)c1cccc1COc1ccn(-c2ccc(Cl)cc2)n1</chem>
Mol. weight [g/mol]:	387.82
CAS:	175013-18-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.05		Crippen Method
logp	4.239		Crippen Method
mcvol	272.950	ml/mol	McGowan Method
rinpol	2967.00		NIST Webbook
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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=C175013180&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

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<https://www.chemeo.com/cid/112-598-4/Pyraclostrobin.pdf>

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