

PYRACLOSTROBINE

Other names:

Carbamic acid,
N-[2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]-N-methoxy-, methyl ester
Carbamic acid,
[2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]methoxy-, methyl ester
N-(2-(((1-(4-chlorophenyl)-1H-pyrazol-3-yl)oxy)methyl)phenyl)-N-methoxycarbamic acid methyl ester
pyraclostrobin
methyl
(2-(((1-(4-chlorophenyl)-1H-pyrazol-3-yl)oxy)methyl)phenyl)(methoxy)carbamate
methyl
[2-[[[1-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]methyl]phenyl]methoxycarbamate
Inchi:

InchiKey:

HZRSNVGNWUDEFX-UHFFFAOYSA-N

Formula:

C19H18ClN3O4

SMILES:

COC(=O)N(OC)c1ccccc1COc1ccn(-c2ccc(Cl)cc2)n1

Mol. weight [g/mol]:

387.82

Physical Properties

Property code	Value	Unit	Source
logp	4.239		Crippen Method
mcvol	272.950	ml/mol	McGowan Method
rinpol	2967.00		NIST Webbook
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tf	333.70	K	Determination and correlation of solubility and thermodynamic properties of pyraclostrobin in pure and binary solvents
tf	333.75	K	Construction and evaluation of ternary solid-liquid phase diagram of pyraclostrobin (form IV) and its intermediate in ethanol and N,N-dimethylformamide

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Determination and correlation of solubility and thermodynamic properties of pyraclostrobin in pure and binary solvents:
<https://www.doi.org/10.1016/j.jct.2016.05.005>

Construction and evaluation of ternary solid-liquid phase diagram of pyraclostrobin (form IV) and its intermediate in ethanol and N,N-dimethylformamide:
<https://www.doi.org/10.1016/j.jct.2018.07.025>

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175013180&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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

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