

# Azoxystrobin

<b>Other names:</b>	Azoxystrobine x Benzeneacetic acid, 2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-«alpha»-(methoxymethylene)-, methyl ester, («alpha»E)- methyl ((E)-2-((6-(2-cyanophenoxy)-4-pyrimidinyl)oxy)-alpha-(methoxymethylene)benzeneacetate methyl (E)-2-(2-((6-(2-cyanophenoxy)pyrimidin-4-yl)oxy)phenyl)-3-methoxyacrylate
<b>Inchi:</b>	InChI=1S/C22H17N3O5/c1-27-13-17(22(26)28-2)16-8-4-6-10-19(16)30-21-11-20(24-14-
<b>InchiKey:</b>	WFDXOXNFNHRHQEC-GHRIWEEISA-N
<b>Formula:</b>	C22H17N3O5
<b>SMILES:</b>	<chem>COC=C(C(=O)OC)c1cccc1Oc1cc(Oc2cccc2C#N)ncn1</chem>
<b>Mol. weight [g/mol]:</b>	403.39
<b>CAS:</b>	131860-33-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	4.093		Crippen Method
mvol	291.650	ml/mol	McGowan Method
rinpol	3083.00		NIST Webbook
tf	387.67	K	Measurement and Correlation of the Solubility of Azoxystrobin in Seven Monosolvents and Two Different Binary Mixed Solvents

## Sources

Measurement and Correlation of the Solubilities of Azoxystrobin, Flutriafol, and Fenprophamid in Subcritical and Supercritical CO<sub>2</sub> Measured by the Static Precise Mass Measuring Method: NIST Webbook.

<https://www.doi.org/10.1021/acs.jced.8b00240>

Crippen Method:

<https://www.doi.org/10.1021/acs.jced.8b00388>

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C131860338&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Measurement and Correlation of the Solubility of Azoxystrobin in Seven Monosolvents and Two Different Binary Mixed Solvents:

<https://www.doi.org/10.1021/acs.jced.7b00669>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>tf:</b>	Normal melting (fusion) point

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