

Prochloraz

Other names:	1H-Imidazole-1-carboxamide, N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]- Ascurit BTS 40542 Mirage N-Propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]-1H-imidazole-1-carboxamide Octave Omega Prelude Sporgon Sportak BTS 40542-7877 DMI KI 835 Mirage (pesticide) cyproconazole
Inchi:	InChI=1S/C15H16Cl3N3O2/c1-2-5-20(15(22)21-6-3-4-19-21)7-8-23-14-12(17)9-11(16)10
InchiKey:	IVCITWHJIOQNBI-UHFFFAOYSA-N
Formula:	C15H16Cl3N3O2
SMILES:	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)n1ccn1
Mol. weight [g/mol]:	376.67
CAS:	68444-81-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	4.602		Crippen Method
mcvol	253.090	ml/mol	McGowan Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook

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=C68444815&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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