

Fenpiclonil

Other names:	4-(2,3-Dichlorophenyl)pyrrole-3-carbonitrile 4-(2,3-Dichlorophenyl)-1H-pyrrole-3-carbonitrile 1H-Pyrrole-3-carbonitrile, 4-(2,3-dichlorophenyl)-
Inchi:	InChI=1S/C11H6Cl2N2/c12-10-3-1-2-8(11(10)13)9-6-15-5-7(9)4-14/h1-3,5-6,15H
InchiKey:	FKLFBQCQQYDUAM-UHFFFAOYSA-N
Formula:	C11H6Cl2N2
SMILES:	N#Cc1c[nH]cc1-c1cccc(Cl)c1Cl
Mol. weight [g/mol]:	237.09
CAS:	74738-17-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	3.378		Crippen Method
mcvol	158.470	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74738173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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