imibenconazole

Other names:	1H-1,2,4-Triazole-1-ethanimidothioic acid, N-(2,4-dichlorophenyl)-, S-[(4-chlorophenyl)methyl] ester
Inchi:	InChI=1S/C17H13Cl3N4S/c18-13-3-1-12(2-4-13)9-25-17(8-24-11-21-10-22-24)23-16-6-5
InchiKey:	AGKSTYPVMZODRV-UHFFFAOYSA-N
Formula:	C17H13Cl3N4S
SMILES:	Clc1ccc(CSC(Cn2cncn2)=Nc2ccc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	411.74
CAS:	86598-92-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.61		Crippen Method
logp	5.902		Crippen Method
mcvol	272.100	ml/mol	McGowan Method
rinpol	3187.00		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=C86598927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices