

# Imibenconazole debenzylated

**Inchi:** InChI=1S/C10H8Cl2N4S/c11-7-1-2-9(8(12)3-7)15-10(17)4-16-6-13-5-14-16/h1-3,5-6H,4H  
**InchiKey:** DMOYSBNHIGDPOM-UHFFFAOYSA-N  
**Formula:** C10H8Cl2N4S  
**SMILES:** S=C(Cn1cncn1)Nc1ccc(Cl)cc1Cl  
**Mol. weight [g/mol]:** 287.17

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	3.024		Crippen Method
mcvol	184.990	ml/mol	McGowan Method
rinpole	2210.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R566586&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpole:** Non-polar retention indices

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