

# Purine, 7-benzyl-2,6-dichloro-

**Inchi:** InChI=1S/C12H8Cl2N4/c13-10-9-11(17-12(14)16-10)15-7-18(9)6-8-4-2-1-3-5-8/h1-5,7H,1  
**InchiKey:** XRCTVEFABOUQNI-UHFFFAOYSA-N  
**Formula:** C12H8Cl2N4  
**SMILES:** Clc1nc(Cl)c2c(ncn2Cc2ccccc2)n1  
**Mol. weight [g/mol]:** 279.12  
**CAS:** 56025-87-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	3.181		Crippen Method
mcvol	181.660	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56025877&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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