

# 2,6-Pyridinedicarbamic acid, 4-chloro-, dibenzyl ester

**Inchi:** InChI=1S/C21H18ClN3O4/c22-17-11-18(24-20(26)28-13-15-7-3-1-4-8-15)23-19(12-17)2  
**InchiKey:** JLBWTVWMYOEKTK-UHFFFAOYSA-N  
**Formula:** C21H18ClN3O4  
**SMILES:** O=C(Nc1cc(Cl)cc(NC(=O)OCc2ccccc2)n1)OCc1ccccc1  
**Mol. weight [g/mol]:** 411.84

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	5.232		Crippen Method
mcvol	292.530	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=B6008382&Units=SI>

## Legend

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

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