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)25

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/ci990307l

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=B6008382&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume