2-Pyridinecarbamic acid, 5,6-diamino-4-[(diphenylmethyl)amino]-, ethyl ester

Inchi: InChI=1S/C21H23N5O2/c1-2-28-21(27)26-17-13-16(18(22)20(23)25-17)24-19(14-9-5-3-6

InchiKey: ZJIORQLFVKLQEZ-UHFFFAOYSA-N

Formula: C21H23N5O2

SMILES: CCOC(=O)Nc1cc(NC(c2ccccc2)c2ccccc2)c(N)c(N)n1

Mol. weight [g/mol]: 377.44

CAS: 38359-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	4.016		Crippen Method
mcvol	292.810	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=C38359681&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume