

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

InChI:  
InChIKey:

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)  
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/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>

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

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