

Pyrido[2,3-b]pyrazine-6-carbamic acid, 8-[(diphenylmethyl)amino]-2,3-diphenyl-, ethyl ester

Inchi:
InchiKey:

InChI=1S/C35H29N5O2/c1-2-42-35(41)38-29-23-28(36-30(24-15-7-3-8-16-24)25-17-9-4

SGPMUSUTOOSHOY-UHFFFAOYSA-N

Formula:

C35H29N5O2

SMILES:

CCOC(=O)Nc1cc(NC(c2ccccc2)c2ccccc2)c2nc(-c3ccccc3)c(-c3ccccc3)nc2n1

Mol. weight [g/mol]:

551.64

CAS:

16335-98-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.26		Crippen Method
logp	8.129		Crippen Method
mcvol	423.090	ml/mol	McGowan Method

Sources

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=C16335981&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/49-700-0/Pyrido-2-3-b-pyrazine-6-carbamic-acid-8-diphenylmethyl-amino-2-3-diphenyl->

Generated by Cheméo on 2024-04-18 09:16:51.696898178 +0000 UTC m=+15721060.617475500.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.