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

Inchi: 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-

InchiKey: 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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume