Pyrido[3,4-b]pyrazine-5,7-dicarbamic acid, 2,3-diphenyl-, diethyl ester

Inchi: InChI=1S/C25H23N5O4/c1-3-33-24(31)28-19-15-18-22(23(27-19)30-25(32)34-4-2)29-21

InchiKey: YEJHPSDVNRGOOU-UHFFFAOYSA-N

Formula: C25H23N5O4

SMILES: CCOC(=O)Nc1cc2nc(-c3ccccc3)c(-c3ccccc3)nc2c(NC(=O)OCC)n1

Mol. weight [g/mol]: 457.48

CAS: 16335-96-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.15		Crippen Method
logp	5.496		Crippen Method
mcvol	337.150	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=C16335969&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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