2,3,10,11-Tetrahydrobenzo[b]dipyrido[3,2,1-de:1,2

Inchi: InChI=1S/C22H16N2O2/c25-17-9-11-23-15-7-3-4-8-16(15)24-12-10-18(26)20-14-6-2-1-5

InchiKey: CJVPWNJSVOPLPU-UHFFFAOYSA-N

Formula: C22H16N2O2

SMILES: O=C1CCN2c3ccccc3N3CCC(=O)c4c3c2c1c1ccccc41

Mol. weight [g/mol]: 340.37

CAS: 100436-05-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	4.602		Crippen Method
mcvol	244.380	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=C100436053&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume