1,3-Diphenyl pyrazolo[3,4-b] pyrazine

Inchi: InChI=1S/C17H12N4/c1-3-7-13(8-4-1)15-16-17(19-12-11-18-16)21(20-15)14-9-5-2-6-10-

InchiKey: VUZFUWYVENKVPR-UHFFFAOYSA-N

Formula: C17H12N4

SMILES: c1ccc(-c2nn(-c3ccccc3)c3nccnc23)cc1

Mol. weight [g/mol]: 272.30

CAS: 93585-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.83		Crippen Method
logp	3.482		Crippen Method
mcvol	203.870	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=C93585230&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume