

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

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