

1,5-dimethyl-3-phenylpyrazole

Inchi:	InChI=1S/C11H12N2/c1-9-8-11(12-13(9)2)10-6-4-3-5-7-10/h3-8H,1-2H3
InchiKey:	AVZWCCJQQCROGD-UHFFFAOYSA-N
Formula:	C11H12N2
SMILES:	Cc1cc(-c2ccccc2)nn1C
Mol. weight [g/mol]:	172.23
CAS:	10250-60-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	2.396		Crippen Method
mcvol	142.590	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10250609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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