

5-Methyl-2H-pyrazole-3-carboxylic acid, 2-phenylhydrazide

Inchi:	InChI=1S/C11H12N4O/c1-8-7-10(14-12-8)11(16)15-13-9-5-3-2-4-6-9/h2-7,13H,1H3,(H,1
InchiKey:	BSFQGLDORMVAOZ-UHFFFAOYSA-N
Formula:	C11H12N4O
SMILES:	Cc1cc(C(=O)NNc2ccccc2)n[nH]1
Mol. weight [g/mol]:	216.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	0.993		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R154613&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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