

5-Methyl-2H-pyrazole-3-carboxylic acid, 1-methyl-2-phenylhydrazide

Inchi: InChI=1S/C12H14N4O/c1-9-8-11(14-13-9)12(17)16(2)15-10-6-4-3-5-7-10/h3-8,15H,1-2H
InchiKey: VKZPHLYTMPNKEN-UHFFFAOYSA-N
Formula: C12H14N4O
SMILES: Cc1cc(C(=O)N(C)Nc2ccccc2)n[nH]1
Mol. weight [g/mol]: 230.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	1.335		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R154579&Units=SI>
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>

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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