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

Inchi: InChI=1S/C11H18N4O/c1-9-8-10(13-12-9)11(16)14(2)15-6-4-3-5-7-15/h8H,3-7H2,1-2H3,

InchiKey: GLLFAVCLMGVCQD-UHFFFAOYSA-N

Formula: C11H18N4O

SMILES: Cc1cc(C(=O)N(C)N2CCCCC2)[nH]n1

Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	0.709		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook

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=R154544&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