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

Inchi: InChI=1S/C9H14N4O/c1-6(2)12-13(4)9(14)8-5-7(3)10-11-8/h5,12H,1H2,2-4H3,(H,10,11)
InchiKey: HHAVUBWVYFUGGD-UHFFFAOYSA-N
Formula: C9H14N4O
SMILES: C=C(C)NN(C)C(=O)c1cc(C)n[nH]1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	0.346		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
rinpol	1554.00		NIST Webbook
rinpol	1554.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R154564&Units=SI
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

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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