

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

Inchi:	InChI=1S/C8H12N4O/c1-5(2)9-12-8(13)7-4-6(3)10-11-7/h4H,1-3H3,(H,10,11)(H,12,13)
InchiKey:	JNJPIJZXUXIIEA-UHFFFAOYSA-N
Formula:	C8H12N4O
SMILES:	CC(C)=NNC(=O)c1cc(C)n[nH]1
Mol. weight [g/mol]:	180.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	0.362		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154608&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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