

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

Inchi:	InChI=1S/C10H16N4O/c1-8-7-9(12-11-8)10(15)13-14-5-3-2-4-6-14/h7H,2-6H2,1H3,(H,1
InchiKey:	VDDZUTDAJOYNNF-UHFFFAOYSA-N
Formula:	C10H16N4O
SMILES:	Cc1cc(C(=O)NN2CCCCC2)n[nH]1
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	0.367		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
rinpol	2137.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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