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

Inchi: InChI=1S/C9H14N4O/c1-7-6-8(11-10-7)9(14)12-13-4-2-3-5-13/h6H,2-5H2,1H3,(H,10,11)
InchiKey: LKCZUEACZROHNE-UHFFFAOYSA-N
Formula: C9H14N4O
SMILES: Cc1cc(C(=O)NN2CCCC2)[nH]n1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	-0.023		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
rinpol	2122.00		NIST Webbook

Sources

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=R154599&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices