2-Pyrazoline, 1,4,5-trimethyl-

Other names: 1,4,5-Trimethyl-«DELTA»[2]-pyrazoline
Inchi: InChI=1S/C6H12N2/c1-5-4-7-8(3)6(5)2/h4-6H,1-3H3
InchiKey: QZXPNIFNBFPOML-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CC1C=NN(C)C1C
Mol. weight [g/mol]: 112.17
CAS: 7423-11-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	0.942		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7423112&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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