2-Pyrazoline, 5-ethyl-1,4-dimethyl-

Other names:	1,4-Dimethyl-5-ethyl-«DELTA»[2]-pyrazoline
	2-Pyrazoline, 1,4-dimethyl-5-ethyl
Inchi:	InChI=1S/C7H14N2/c1-4-7-6(2)5-8-9(7)3/h5-7H,4H2,1-3H3
InchiKey:	LSAFIEKJCBNDJB-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CCC1C(C)C=NN1C
Mol. weight [g/mol]:	126.20
CAS:	14339-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	1.332		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
rinpol	874.00		NIST Webbook
rinpol	874.00		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=C14339232&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

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