

1H-Pyrazole, 3-ethyl-4,5-dihydro-1,4-dimethyl-

Other names:	1,4-Dimethyl-3-ethyl-«DELTA»[2]-pyrazoline 2-Pyrazoline, 1,4-dimethyl-3-ethyl
Inchi:	InChI=1S/C7H14N2/c1-4-7-6(2)5-9(3)8-7/h6H,4-5H2,1-3H3
InchiKey:	VEXJHDVLCQKJJU-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CCC1=NN(C)CC1C
Mol. weight [g/mol]:	126.20
CAS:	75011-91-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Crippen Method
logp	1.334		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
rinpol	943.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C75011915&Units=SI

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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