

2-Pyrazoline, 1-isopropyl-5-methyl-

Other names:	5-Methyl-1-isopropyl-«DELTA»[2]-pyrazoline 1-Isopropyl-5-methyl-4,5-dihydro-1H-pyrazole 1-Isopropyl-5-methyl-2-pyrazoline
Inchi:	InChI=1S/C7H14N2/c1-6(2)9-7(3)4-5-8-9/h5-7H,4H2,1-3H3
InchiKey:	DUOUFHCFRWDSBE-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CC(C)N1N=CCC1C
Mol. weight [g/mol]:	126.20
CAS:	26964-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	1.475		Crippen Method
mcvol	114.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26964545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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