

2-Pyrazoline, 1,3,4-trimethyl-

Other names:	1,3,4-Trimethyl-«DELTA»[2]-pyrazoline 1,3,4-Trimethyl-2-pyrazoline
Inchi:	InChI=1S/C6H12N2/c1-5-4-8(3)7-6(5)2/h5H,4H2,1-3H3
InchiKey:	UWCOGVAFZZBWAT-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	CC1=NN(C)CC1C
Mol. weight [g/mol]:	112.17
CAS:	14044-41-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.71		Crippen Method
logp	0.944		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rinpol	857.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14044418&Units=SI
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

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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