

3H-Pyrazol-3-one, 2,4-dihydro-2,5-dimethyl-

Other names:	2-Pyrazolin-5-one, 1,3-dimethyl- 1,3-Dimethyl-5-pyrazolinone 1,3-Dimethyl-5-pyrazolone 2,4-dihydro-2,5-dimethyl-3H-pyrazol-3-one
Inchi:	InChI=1S/C5H8N2O/c1-4-3-5(8)7(2)6-4/h3H2,1-2H3
InchiKey:	NDELSWXIAJLWOU-UHFFFAOYSA-N
Formula:	C5H8N2O
SMILES:	CC1=NN(C)C(=O)C1
Mol. weight [g/mol]:	112.13
CAS:	2749-59-9

Physical Properties

Property code	Value	Unit	Source
ie	8.65 ± 0.05	eV	NIST Webbook
log10ws	-0.31		Crippen Method
logp	0.224		Crippen Method
mcvol	87.680	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2749599&Units=SI

Legend

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

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