

# 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl-

Other names:

1-Phenyl-3-methyl-2-pyrazolin-5-one  
1-Phenyl-3-methyl-5-pyrazolone  
1-Phenyl-3-methylpyrazolone  
1-Phenyl-3-methylpyrazolone-5  
1-phenyl-3-methyl-1H-4,5-dihydropyrazol-5-one  
2,4-Dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one  
2-Pyrazolin-5-one, 3-methyl-1-phenyl-  
3-Methyl-1-phenyl-2-pyrazolin-5-one  
3-Methyl-1-phenyl-5-pyrazolone  
3-Methyl-1-phenylpyrazol-5(4H)-one  
3-Methyl-1-phenylpyrazol-5-one  
3-Methyl-1-phenylpyrazolin-5-one  
4,5-dihydro-3-methyl-5-oxo-1-phenylpyrazole  
5-Pyrazolone, 3-methyl-1-phenyl-  
5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one  
C.I. Developer 1  
Developer Z  
Edaravone  
Methylphenylpyrazolone  
NCI-C03952  
NSC-12  
NSC-26139  
NSC-2629  
Norantipyrine  
Norphenazone  
Radicut  
InChI=1S/C10H10N2O/c1-8-7-10(13)12(11-8)9-5-3-2-4-6-9/h2-6H,7H2,1H3  
QELUYTUMUWHWMC-UHFFFAOYSA-N  
C10H10N2O  
CC1=NN(c2ccccc2)C(=O)C1  
174.20  
89-25-8

**Inchi:**  
**InchiKey:**  
**Formula:**  
**SMILES:**  
**Mol. weight [g/mol]:**  
**CAS:**

## Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook

ie	8.00 ± 0.05	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.799		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
tt	400.15	K	Co-solvence phenomenon and thermodynamic properties of edaravone in pure and mixed solvents

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	560.20	K	35.30	NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Co-solvence phenomenon and thermodynamic properties of edaravone in pure and mixed solvents:	<a href="https://www.doi.org/10.1016/j.jct.2019.06.018">https://www.doi.org/10.1016/j.jct.2019.06.018</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C89258&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89258&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tt:</b>	Triple Point Temperature

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