

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

Other names:	1-Fenyl-3-methyl-2-pyrazolin-5-on
	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:	InChI=1S/C10H10N2O/c1-8-7-10(13)12(11-8)9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	QELUYTUMUWHWMC-UHFFFAOYSA-N
Formula:	C10H10N2O
SMILES:	CC1=NN(c2ccccc2)C(=O)C1
Mol. weight [g/mol]:	174.20
CAS:	89-25-8

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-solvent 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Co-solvent phenomenon and thermodynamic properties of edaravone in pure and mixed solvents:	https://www.doi.org/10.1016/j.jct.2019.06.018
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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