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-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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Co-solvence 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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89258&Units=SI

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