

Picrolonic acid

Other names:

3H-Pyrazol-3-one, 1,4-dihydro-5-methyl-4-nitro-2-(4-nitrophenyl)-
2-Pyrazolin-5-one, 3-methyl-4-nitro-1-(p-nitrophenyl)-
3-Methyl-4-nitro-1-(p-nitrophenyl)-2-pyrazolin-5-one
3-methyl-4-nitro-1-p-nitrophenyl-5-pyrazolone

Inchi:

InChI=1S/C10H8N4O5/c1-6-9(14(18)19)10(15)12(11-6)7-2-4-8(5-3-7)13(16)17/h2-5,9H,1

InchiKey:

OVFUUSPKWADLNJ-UHFFFAOYSA-N

Formula:

C10H8N4O5

SMILES:

CC1=NN(c2ccc([N+](=O)[O-])cc2)C(=O)C1[N+](=O)[O-]

Mol. weight [g/mol]:

264.19

CAS:

550-74-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	0.963		Crippen Method
mcvol	169.210	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=C550743&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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