

# 1-methyl-3,5-dinitropyrazole

**Inchi:** InChI=1S/C4H4N4O4/c1-6-4(8(11)12)2-3(5-6)7(9)10/h2H,1H3  
**InchiKey:** UWSPNIADTGDCIW-UHFFFAOYSA-N  
**Formula:** C4H4N4O4  
**SMILES:** Cn1nc([N+](=O)[O-])cc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 172.10  
**CAS:** 32683-48-0

## Physical Properties

Property code	Value	Unit	Source
affp	788.80	kJ/mol	NIST Webbook
basg	757.00	kJ/mol	NIST Webbook
log10ws	-3.83		Crippen Method
logp	0.236		Crippen Method
mcvol	102.560	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](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=C32683480&Units=SI>

## Legend

**affp:** Proton affinity  
**basg:** Gas basicity  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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