

# 3-Penten-2-one, 2,4-dinitrophenylhydrazone

**Inchi:** InChI=1S/C11H12N4O4/c1-3-4-8(2)12-13-10-6-5-9(14(16)17)7-11(10)15(18)19/h3-7,13H  
**InchiKey:** WSGQQBRVKFRFJN-ALUKSYHCSA-N  
**Formula:** C11H12N4O4  
**SMILES:** CC=CC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 264.24  
**CAS:** 4938-74-3

## Physical Properties

Property code	Value	Unit	Source
hf	164.82	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	2.867		Crippen Method
mcvol	188.290	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	922.29	K	Joback Method
tc	1191.59	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4938743&Units=SI>  
**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)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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