

# benzaldehyde oxime, 2-hydroxy, 3-nitro, 5-(1,1,3,3-tetramethylbutyl)

**Inchi:** InChI=1S/C15H22N2O4/c1-14(2,3)9-15(4,5)11-6-10(8-16-19)13(18)12(7-11)17(20)21/h6  
**InchiKey:** UAWZWSYAHLOIEX-UHFFFAOYSA-N  
**Formula:** C15H22N2O4  
**SMILES:** CC(C)(C)CC(C)(C)c1cc(C=NO)c(O)c([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 294.35

## Physical Properties

Property code	Value	Unit	Source
hf	-414.92	kJ/mol	Joback Method
hvap	99.59	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.822		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	974.10	K	Joback Method
tc	1216.17	K	Joback 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)  
**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R256947&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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