

# 2,4,4-Trimethyl-2-pentanol, nitrite

**Inchi:** InChI=1S/C8H17NO2/c1-7(2,3)6-8(4,5)11-9-10/h6H2,1-5H3  
**InchiKey:** OVNLRVZDVRUHRQ-UHFFFAOYSA-N  
**Formula:** C8H17NO2  
**SMILES:** CC(C)(C)CC(C)(C)ON=O  
**Mol. weight [g/mol]:** 159.23

## Physical Properties

Property code	Value	Unit	Source
hf	-526.36	kJ/mol	Joback Method
hvap	42.32	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.899		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	461.80	K	Joback Method
tc	648.22	K	Joback Method

## Sources

**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=R311490&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)

## Legend

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

**mcvol:** McGowan's characteristic volume  
**pc:** Critical Pressure  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature

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