

# 2-Methyl-3-nitrophenol

<b>Other names:</b>	Phenol, 2-methyl-3-nitro- 3-Nitro-O-cresol 2-Hydroxy-6-nitrotoluene
<b>Inchi:</b>	InChI=1S/C7H7NO3/c1-5-6(8(10)11)3-2-4-7(5)9/h2-4,9H,1H3
<b>InchiKey:</b>	GAKLFAZBKQGUBO-UHFFFAOYSA-N
<b>Formula:</b>	C7H7NO3
<b>SMILES:</b>	<chem>Cc1c(O)cccc1[N+](=O)[O-]</chem>
<b>Mol. weight [g/mol]:</b>	153.14
<b>CAS:</b>	5460-31-1

## Physical Properties

Property code	Value	Unit	Source
gf	-8.23	kJ/mol	Joback Method
hf	-150.82	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.609		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	623.68	K	Joback Method
tc	883.67	K	Joback Method
tf	462.92	K	Joback Method
vc	0.367	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.28	J/molxK	623.68	Joback Method
cpg	271.81	J/molxK	667.01	Joback Method
cpg	280.56	J/molxK	710.34	Joback Method
cpg	288.66	J/molxK	753.67	Joback Method
cpg	296.21	J/molxK	797.01	Joback Method
cpg	303.32	J/molxK	840.34	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5460311&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5460311&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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