

# Phenol, 4-(1-methylpentyl)-2-nitro

<b>Inchi:</b>	InChI=1S/C12H17NO3/c1-3-4-5-9(2)10-6-7-12(14)11(8-10)13(15)16/h6-9,14H,3-5H2,1-2
<b>InchiKey:</b>	DPTMPFVIJHQGLP-UHFFFAOYSA-N
<b>Formula:</b>	C12H17NO3
<b>SMILES:</b>	CCCCC(C)c1ccc(O)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	223.27

## Physical Properties

Property code	Value	Unit	Source
gf	31.43	kJ/mol	Joback Method
hf	-259.30	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.594		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	737.64	K	Joback Method
tc	975.34	K	Joback Method
tf	504.27	K	Joback Method
vc	0.641	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.19	J/molxK	737.64	Joback Method
cpg	521.85	J/molxK	777.26	Joback Method
cpg	534.66	J/molxK	816.87	Joback Method
cpg	546.75	J/molxK	856.49	Joback Method
cpg	558.20	J/molxK	896.11	Joback Method
cpg	569.14	J/molxK	935.72	Joback Method
cpg	579.66	J/molxK	975.34	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R58810&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R58810&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>

# 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>h vap:</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>r in pol:</b>	Non-polar retention indices
<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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