

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

<b>Inchi:</b>	InChI=1S/C11H15NO3/c1-3-8(4-2)10-7-9(12(14)15)5-6-11(10)13/h5-8,13H,3-4H2,1-2H3
<b>InchiKey:</b>	QNRJXDZNLJOGBQ-UHFFFAOYSA-N
<b>Formula:</b>	C11H15NO3
<b>SMILES:</b>	CCC(CC)c1cc([N+](=O)[O-])ccc1O
<b>Mol. weight [g/mol]:</b>	209.24

## Physical Properties

Property code	Value	Unit	Source
gf	23.01	kJ/mol	Joback Method
hf	-238.66	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	72.23	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.204		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinsol	1830.00		NIST Webbook
tb	714.76	K	Joback Method
tc	957.31	K	Joback Method
tf	493.00	K	Joback Method
vc	0.586	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.33	J/mol×K	714.76	Joback Method
cpg	469.42	J/mol×K	755.18	Joback Method
cpg	481.65	J/mol×K	795.61	Joback Method
cpg	493.15	J/mol×K	836.03	Joback Method
cpg	504.02	J/mol×K	876.46	Joback Method
cpg	514.36	J/mol×K	916.88	Joback Method
cpg	524.29	J/mol×K	957.31	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=R58646&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R58646&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>mccvol:</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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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