

# 2-Methoxy-4-(2-nitropropenyl)phenol

<b>Inchi:</b>	InChI=1S/C10H11NO4/c1-7(11(13)14)5-8-3-4-9(12)10(6-8)15-2/h3-6,12H,1-2H3/b7-5-
<b>InchiKey:</b>	FDLWTEUMNRJFCS-ALCCZGGFSA-N
<b>Formula:</b>	C10H11NO4
<b>SMILES:</b>	COc1cc(C=C(C)[N+](=O)[O-])ccc1O
<b>Mol. weight [g/mol]:</b>	209.20

## Physical Properties

Property code	Value	Unit	Source
gf	-16.30	kJ/mol	Joback Method
hf	-237.53	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	72.84	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.038		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	718.78	K	Joback Method
tc	971.73	K	Joback Method
tf	499.92	K	Joback Method
vc	0.534	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.56	J/molxK	718.78	Joback Method
cpg	415.98	J/molxK	760.94	Joback Method
cpg	426.65	J/molxK	803.10	Joback Method
cpg	436.69	J/molxK	845.26	Joback Method
cpg	446.21	J/molxK	887.42	Joback Method
cpg	455.33	J/molxK	929.57	Joback Method
cpg	464.15	J/molxK	971.73	Joback Method

# Sources

<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>
<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=B6006708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006708&amp;Units=SI</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>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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