

# 4-(2-Nitrophenyl)but-3-en-2-one

<b>Inchi:</b>	InChI=1S/C10H9NO3/c1-8(12)6-7-9-4-2-3-5-10(9)11(13)14/h2-7H,1H3/b7-6+
<b>InchiKey:</b>	FRPAGLRAZLFTGW-VOTSOKGWSA-N
<b>Formula:</b>	C10H9NO3
<b>SMILES:</b>	CC(=O)C=Cc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	191.18
<b>CAS:</b>	20766-40-9

## Physical Properties

Property code	Value	Unit	Source
gf	122.95	kJ/mol	Joback Method
hf	-30.79	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-3.06		Crippen Method
logp	2.197		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	669.73	K	Joback Method
tc	921.09	K	Joback Method
tf	429.86	K	Joback Method
vc	0.555	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.57	J/molxK	669.73	Joback Method
cpg	360.22	J/molxK	711.62	Joback Method
cpg	370.90	J/molxK	753.52	Joback Method
cpg	380.71	J/molxK	795.41	Joback Method
cpg	389.70	J/molxK	837.30	Joback Method
cpg	397.97	J/molxK	879.20	Joback Method
cpg	405.57	J/molxK	921.09	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20766409&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20766409&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>ie:</b>	Ionization energy
<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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