

# 2-nitrophenyl acetate

<b>Inchi:</b>	InChI=1S/C8H7NO4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3
<b>InchiKey:</b>	MRCKRGSNLOHYRA-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO4
<b>SMILES:</b>	CC(=O)Oc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	181.15
<b>CAS:</b>	610-69-5

## Physical Properties

Property code	Value	Unit	Source
gf	-79.11	kJ/mol	Joback Method
hf	-238.95	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.520		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	642.23	K	Joback Method
tc	889.97	K	Joback Method
tf	434.63	K	Joback Method
vc	0.481	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.26	J/molxK	642.23	Joback Method
cpg	308.88	J/molxK	683.52	Joback Method
cpg	318.68	J/molxK	724.81	Joback Method
cpg	327.67	J/molxK	766.10	Joback Method
cpg	335.88	J/molxK	807.39	Joback Method
cpg	343.31	J/molxK	848.68	Joback Method
cpg	349.99	J/molxK	889.97	Joback Method
hvapt	71.10	kJ/mol	449.50	NIST Webbook

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	1.50	NIST Webbook

## Sources

<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=C610695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C610695&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>

## 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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