

# 4-Nitrophenoxyacetonitrile

<b>Inchi:</b>	InChI=1S/C8H6N2O3/c9-5-6-13-8-3-1-7(2-4-8)10(11)12/h1-4H,6H2
<b>InchiKey:</b>	HFRYXZNUOFIXGS-UHFFFAOYSA-N
<b>Formula:</b>	C8H6N2O3
<b>SMILES:</b>	N#CCOc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	178.14
<b>CAS:</b>	33901-46-1

## Physical Properties

Property code	Value	Unit	Source
gf	182.99	kJ/mol	Joback Method
hf	38.51	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	65.82	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.497		Crippen Method
mcvol	124.490	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	690.44	K	Joback Method
tc	943.89	K	Joback Method
tf	449.69	K	Joback Method
vc	0.501	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.29	J/molxK	690.44	Joback Method
cpg	310.51	J/molxK	732.68	Joback Method
cpg	318.95	J/molxK	774.92	Joback Method
cpg	326.64	J/molxK	817.16	Joback Method
cpg	333.59	J/molxK	859.41	Joback Method
cpg	339.83	J/molxK	901.65	Joback Method
cpg	345.38	J/molxK	943.89	Joback Method

# 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=C33901461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33901461&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>

# 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>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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