

# Methyl 4-nitrophenylacetate

<b>Inchi:</b>	InChI=1S/C9H9NO4/c1-14-9(11)6-7-2-4-8(5-3-7)10(12)13/h2-5H,6H2,1H3
<b>InchiKey:</b>	PQRGTRBYCFLHKY-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO4
<b>SMILES:</b>	<chem>COC(=O)Cc1ccc([N+](=O)[O-])cc1</chem>
<b>Mol. weight [g/mol]:</b>	195.17
<b>CAS:</b>	2945-08-6

## Physical Properties

Property code	Value	Unit	Source
gf	-70.69	kJ/mol	Joback Method
hf	-259.59	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.310		Crippen Method
mvol	138.770	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	665.11	K	Joback Method
tc	907.46	K	Joback Method
tf	445.90	K	Joback Method
vc	0.537	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.96	J/mol×K	665.11	Joback Method
cpg	357.42	J/mol×K	705.50	Joback Method
cpg	367.99	J/mol×K	745.89	Joback Method
cpg	377.72	J/mol×K	786.28	Joback Method
cpg	386.61	J/mol×K	826.67	Joback Method
cpg	394.70	J/mol×K	867.07	Joback Method
cpg	401.99	J/mol×K	907.46	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2945086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2945086&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>hvp:</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>rinp:</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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