

# Phenyl-4-nitrophenylacetic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C15H13NO4/c1-20-15(17)14(11-5-3-2-4-6-11)12-7-9-13(10-8-12)16(18)19/h2-
<b>InchiKey:</b>	JMRXEYLVZUDJR-UHFFFAOYSA-N
<b>Formula:</b>	C15H13NO4
<b>SMILES:</b>	<chem>COC(=O)C(c1ccccc1)c1ccc([N+](=O)[O-])cc1</chem>
<b>Mol. weight [g/mol]:</b>	271.27

## Physical Properties

Property code	Value	Unit	Source
gf	89.80	kJ/mol	Joback Method
hf	-152.18	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.900		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpola	2205.00		NIST Webbook
rinpola	2205.00		NIST Webbook
tb	828.63	K	Joback Method
tc	1089.25	K	Joback Method
tf	524.94	K	Joback Method
vc	0.759	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.92	J/mol×K	828.63	Joback Method
cpg	577.56	J/mol×K	872.07	Joback Method
cpg	588.88	J/mol×K	915.50	Joback Method
cpg	598.95	J/mol×K	958.94	Joback Method
cpg	607.85	J/mol×K	1002.38	Joback Method
cpg	615.64	J/mol×K	1045.82	Joback Method
cpg	622.41	J/mol×K	1089.25	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=R190139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190139&amp;Units=SI</a>
<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>

# 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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