

# 4-Nitrobenzoic acid, 3-methylbut-2-enyl ester

<b>Inchi:</b>	InChI=1S/C12H13NO4/c1-9(2)7-8-17-12(14)10-3-5-11(6-4-10)13(15)16/h3-7H,8H2,1-2H
<b>InchiKey:</b>	MBCPNFHFYXLONQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H13NO4
<b>SMILES:</b>	CC(C)=CCOC(=O)c1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	235.24

## Physical Properties

Property code	Value	Unit	Source
gf	26.24	kJ/mol	Joback Method
hf	-214.08	kJ/mol	Joback Method
hfus	33.53	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.718		Crippen Method
mcvol	176.740	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinsol	1811.00		NIST Webbook
tb	737.79	K	Joback Method
tc	978.69	K	Joback Method
tf	460.67	K	Joback Method
vc	0.686	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.70	J/mol×K	737.79	Joback Method
cpg	485.49	J/mol×K	777.94	Joback Method
cpg	497.28	J/mol×K	818.09	Joback Method
cpg	508.14	J/mol×K	858.24	Joback Method
cpg	518.11	J/mol×K	898.39	Joback Method
cpg	527.25	J/mol×K	938.54	Joback Method
cpg	535.61	J/mol×K	978.69	Joback Method

# Sources

<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=U299265&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299265&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>
<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>

# 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>rinpola:</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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