

# Ethyl p-nitrophenyl carbonate

<b>Other names:</b>	Carbonic acid, ethyl 4-nitrophenyl ester
<b>Inchi:</b>	InChI=1S/C9H9NO5/c1-2-14-9(11)15-8-5-3-7(4-6-8)10(12)13/h3-6H,2H2,1H3
<b>InchiKey:</b>	OFJLSOXXIMLDDL-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO5
<b>SMILES:</b>	CCOC(=O)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	211.17
<b>CAS:</b>	6132-45-2

## Physical Properties

Property code	Value	Unit	Source
gf	-175.69	kJ/mol	Joback Method
hf	-391.81	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.130		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1658.00		NIST Webbook
tb	687.53	K	Joback Method
tc	926.11	K	Joback Method
tf	468.13	K	Joback Method
vc	0.555	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.14	J/molxK	687.53	Joback Method
cpg	380.40	J/molxK	727.29	Joback Method
cpg	390.79	J/molxK	767.06	Joback Method
cpg	400.33	J/molxK	806.82	Joback Method
cpg	409.00	J/molxK	846.58	Joback Method
cpg	416.80	J/molxK	886.35	Joback Method
cpg	423.74	J/molxK	926.11	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=C6132452&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6132452&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>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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