

# Benzoic acid, 2-amino-, 2-propenyl ester

<b>Other names:</b>	Anthranilic acid, allyl ester Allyl anthranilate 2-Propenyl 2-aminobenzoate 2-Propen-1-yl anthranilate
<b>Inchi:</b>	InChI=1S/C10H11NO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h2-6H,1,7,11H2
<b>InchiKey:</b>	UCANFCXAKYMFGA-UHFFFAOYSA-N
<b>Formula:</b>	C10H11NO2
<b>SMILES:</b>	<chem>C=CCOC(=O)c1ccccc1N</chem>
<b>Mol. weight [g/mol]:</b>	177.20
<b>CAS:</b>	7493-63-2

## Physical Properties

Property code	Value	Unit	Source
gf	56.47	kJ/mol	Joback Method
hf	-110.25	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.612		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	605.36	K	Joback Method
tc	832.15	K	Joback Method
tf	395.06	K	Joback Method
vc	0.521	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.24	J/molxK	605.36	Joback Method
cpg	348.55	J/molxK	643.16	Joback Method
cpg	360.07	J/molxK	680.96	Joback Method
cpg	370.81	J/molxK	718.75	Joback Method
cpg	380.79	J/molxK	756.55	Joback Method

cpg	390.05	J/mol×K	794.35	Joback Method
cpg	398.60	J/mol×K	832.15	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=C7493632&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7493632&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>hvac:</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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