

# Benzoic acid, 2-amino-, phenyl ester

<b>Other names:</b>	phenyl anthranilate
<b>Inchi:</b>	InChI=1S/C13H11NO2/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9H,14H2
<b>InchiKey:</b>	ZBFSYQBEXZGTAX-UHFFFAOYSA-N
<b>Formula:</b>	C13H11NO2
<b>SMILES:</b>	<chem>Nc1cccc1C(=O)Oc1cccc1</chem>
<b>Mol. weight [g/mol]:</b>	213.23
<b>CAS:</b>	10268-69-6

## Physical Properties

Property code	Value	Unit	Source
gf	106.30	kJ/mol	Joback Method
hf	-61.07	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	69.54	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.488		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	704.00	K	Joback Method
tc	958.33	K	Joback Method
tf	457.05	K	Joback Method
vc	0.601	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.53	J/molxK	704.00	Joback Method
cpg	435.97	J/molxK	746.39	Joback Method
cpg	448.22	J/molxK	788.78	Joback Method
cpg	459.34	J/molxK	831.17	Joback Method
cpg	469.38	J/molxK	873.55	Joback Method
cpg	478.39	J/molxK	915.94	Joback Method
cpg	486.42	J/molxK	958.33	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C10268696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10268696&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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/32-636-0/Benzoic-acid-2-amino-phenyl-ester.pdf>

Generated by Cheméo on 2024-04-29 09:59:20.013782213 +0000 UTC m=+16674008.934359525.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.