

# Benzoic acid, 2-amino-, 1-methylethyl ester

<b>Other names:</b>	Anthranilic acid, isopropyl ester Isopropyl anthranilate Isopropyl 2-aminobenzoate
<b>Inchi:</b>	InChI=1S/C10H13NO2/c1-7(2)13-10(12)8-5-3-4-6-9(8)11/h3-7H,11H2,1-2H3
<b>InchiKey:</b>	XKOZHFJYXAQZJX-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NO2
<b>SMILES:</b>	CC(C)OC(=O)c1ccccc1N
<b>Mol. weight [g/mol]:</b>	179.22
<b>CAS:</b>	18189-02-1

## Physical Properties

Property code	Value	Unit	Source
gf	-33.81	kJ/mol	Joback Method
hf	-240.96	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.834		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	608.24	K	Joback Method
tc	835.08	K	Joback Method
tf	381.82	K	Joback Method
vc	0.534	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.55	J/mol×K	608.24	Joback Method
cpg	370.93	J/mol×K	646.05	Joback Method
cpg	383.46	J/mol×K	683.85	Joback Method
cpg	395.16	J/mol×K	721.66	Joback Method

cpg	406.06	J/mol×K	759.47	Joback Method
cpg	416.18	J/mol×K	797.28	Joback Method
cpg	425.52	J/mol×K	835.08	Joback Method

## Sources

<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=C18189021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18189021&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpol:</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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