

# Anthranilic acid, n-(o-nitrophenyl)-

<b>Inchi:</b>	InChI=1S/C13H10N2O4/c16-13(17)9-5-1-2-6-10(9)14-11-7-3-4-8-12(11)15(18)19/h1-8,1
<b>InchiKey:</b>	FJNZXTAFUISVCI-UHFFFAOYSA-N
<b>Formula:</b>	C13H10N2O4
<b>SMILES:</b>	O=C(O)c1ccccc1Nc1cccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	258.23
<b>CAS:</b>	5933-35-7

## Physical Properties

Property code	Value	Unit	Source
gf	123.34	kJ/mol	Joback Method
hf	-83.63	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	96.86	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.037		Crippen Method
mvol	181.350	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	908.22	K	Joback Method
tc	1154.92	K	Joback Method
tf	621.17	K	Joback Method
vc	0.690	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.07	J/mol×K	908.22	Joback Method
cpg	528.48	J/mol×K	949.34	Joback Method
cpg	536.05	J/mol×K	990.45	Joback Method
cpg	542.84	J/mol×K	1031.57	Joback Method
cpg	548.94	J/mol×K	1072.69	Joback Method
cpg	554.41	J/mol×K	1113.80	Joback Method
cpg	559.32	J/mol×K	1154.92	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=C5933357&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5933357&amp;Units=SI</a>
<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>

# 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

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