

# 4-Nitrophenylanthranilate

<b>Inchi:</b>	InChI=1S/C13H10N2O4/c14-12-4-2-1-3-11(12)13(16)19-10-7-5-9(6-8-10)15(17)18/h1-8H
<b>InchiKey:</b>	IFHJJPYCVMFLMB-UHFFFAOYSA-N
<b>Formula:</b>	C13H10N2O4
<b>SMILES:</b>	<chem>Nc1cccc1C(=O)Oc1ccc([N+](=O)[O-])cc1</chem>
<b>Mol. weight [g/mol]:</b>	258.23
<b>CAS:</b>	19176-60-4

## Physical Properties

Property code	Value	Unit	Source
gf	132.22	kJ/mol	Joback Method
hf	-83.30	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.396		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	860.82	K	Joback Method
tc	1131.64	K	Joback Method
tf	613.18	K	Joback Method
vc	0.682	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.91	J/molxK	860.82	Joback Method
cpg	519.14	J/molxK	905.96	Joback Method
cpg	528.15	J/molxK	951.09	Joback Method
cpg	536.00	J/molxK	996.23	Joback Method
cpg	542.74	J/molxK	1041.37	Joback Method
cpg	548.45	J/molxK	1086.50	Joback Method
cpg	553.18	J/molxK	1131.64	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19176604&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19176604&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>
<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>

# 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>h vap:</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>m cvol:</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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