

# Aniline, 4-nitro-3-phenylthio-

<b>Inchi:</b>	InChI=1S/C12H10N2O2S/c13-9-6-7-11(14(15)16)12(8-9)17-10-4-2-1-3-5-10/h1-8H,13H2
<b>InchiKey:</b>	KTUGOFDZPGGYLI-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N2O2S
<b>SMILES:</b>	<chem>Nc1ccc([N+](=O)[O-])c(Sc2ccccc2)c1</chem>
<b>Mol. weight [g/mol]:</b>	246.28
<b>CAS:</b>	28819-80-9

## Physical Properties

Property code	Value	Unit	Source
gf	390.84	kJ/mol	Joback Method
hf	224.01	kJ/mol	Joback Method
hfus	34.83	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.328		Crippen Method
mcvol	176.170	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	830.43	K	Joback Method
tc	1124.45	K	Joback Method
tf	564.15	K	Joback Method
vc	0.656	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.87	J/molxK	830.43	Joback Method
cpg	482.06	J/molxK	879.43	Joback Method
cpg	491.91	J/molxK	928.44	Joback Method
cpg	500.51	J/molxK	977.44	Joback Method
cpg	507.96	J/molxK	1026.45	Joback Method
cpg	514.35	J/molxK	1075.45	Joback Method
cpg	519.78	J/molxK	1124.45	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C28819809&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28819809&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

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