

# Ethanethioamide, N-phenyl-

<b>Other names:</b>	Acetanilide, thio- N-Phenylthioacetamide Thioacetanilide USAF ek-1902
<b>Inchi:</b>	InChI=1S/C8H9NS/c1-7(10)9-8-5-3-2-4-6-8/h2-6H,1H3,(H,9,10)
<b>InchiKey:</b>	MWCGLTCRJFXKR-UHFFFAOYSA-N
<b>Formula:</b>	C8H9NS
<b>SMILES:</b>	CC(=S)Nc1ccccc1
<b>Mol. weight [g/mol]:</b>	151.23
<b>CAS:</b>	637-53-6

## Physical Properties

Property code	Value	Unit	Source
gf	335.34	kJ/mol	Joback Method
hf	228.05	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-2.75		Crippen Method
logp	2.446		Crippen Method
mvol	121.850	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	529.33	K	Joback Method
tc	770.26	K	Joback Method
tf	293.27	K	Joback Method
vc	0.447	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.37	J/mol×K	529.33	Joback Method
cpg	261.48	J/mol×K	569.49	Joback Method
cpg	272.58	J/mol×K	609.64	Joback Method
cpg	282.75	J/mol×K	649.80	Joback Method

cpg	292.07	J/mol×K	689.95	Joback Method
cpg	300.64	J/mol×K	730.11	Joback Method
cpg	308.55	J/mol×K	770.26	Joback Method

## Sources

<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>
<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=C637536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C637536&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>ie:</b>	Ionization energy
<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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