

# 4-Acetylphenylisothiocyanate

<b>Other names:</b>	Phenylisothiocyanate, 4-acetyl
<b>Inchi:</b>	InChI=1S/C9H7NOS/c1-7(11)8-2-4-9(5-3-8)10-6-12/h2-5H,1H3
<b>InchiKey:</b>	KAKXOESNHIUYJT-UHFFFAOYSA-N
<b>Formula:</b>	C9H7NOS
<b>SMILES:</b>	CC(=O)c1ccc(N=C=S)cc1
<b>Mol. weight [g/mol]:</b>	177.22
<b>CAS:</b>	2131-57-9

## Physical Properties

Property code	Value	Unit	Source
hf	167.46	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.623		Crippen Method
mcvol	133.210	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	636.80	K	Joback Method
tc	898.72	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131579&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131579&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>
<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>hf:</b>	Enthalpy of formation 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

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