

# Ethanethioic acid, S-(4-methylphenyl) ester

<b>Other names:</b>	S-(4-Methylphenyl) ethanethioate p-Thiocresol, S-acetyl- S-p-Tolyl thioacetate
<b>Inchi:</b>	InChI=1S/C9H10OS/c1-7-3-5-9(6-4-7)11-8(2)10/h3-6H,1-2H3
<b>InchiKey:</b>	XSQUNQSLEIFIHF-UHFFFAOYSA-N
<b>Formula:</b>	C9H10OS
<b>SMILES:</b>	CC(=O)Sc1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	166.24
<b>CAS:</b>	10436-83-6

## Physical Properties

Property code	Value	Unit	Source
gf	31.88	kJ/mol	Joback Method
hf	-74.74	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.634		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpola	1374.50		NIST Webbook
rinpola	1374.50		NIST Webbook
tb	559.63	K	Joback Method
tc	800.44	K	Joback Method
tf	314.46	K	Joback Method
vc	0.491	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.71	J/mol×K	559.63	Joback Method
cpg	293.43	J/mol×K	599.76	Joback Method
cpg	305.31	J/mol×K	639.90	Joback Method
cpg	316.36	J/mol×K	680.03	Joback Method

cpg	326.60	J/mol×K	720.17	Joback Method
cpg	336.07	J/mol×K	760.30	Joback Method
cpg	344.78	J/mol×K	800.44	Joback Method

## Sources

<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=C10436836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10436836&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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>rinpol:</b>	Non-polar retention indices
<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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