

# Benzenemethanethiol, 4-methyl-

<b>Other names:</b>	p-Xylene-alpha-thiol p-xylene-«alpha»-thiol
<b>Inchi:</b>	InChI=1S/C8H10S/c1-7-2-4-8(6-9)5-3-7/h2-5,9H,6H2,1H3
<b>InchiKey:</b>	AGFYZLVFPSGUIX-UHFFFAOYSA-N
<b>Formula:</b>	C8H10S
<b>SMILES:</b>	Cc1ccc(CS)cc1
<b>Mol. weight [g/mol]:</b>	138.23
<b>CAS:</b>	4498-99-1

## Physical Properties

Property code	Value	Unit	Source
gf	148.65	kJ/mol	Joback Method
hf	55.09	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	43.08	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.425		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	476.96	K	Joback Method
tc	713.39	K	Joback Method
tf	255.32	K	Joback Method
vc	0.429	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.48	J/molxK	476.96	Joback Method
cpg	234.25	J/molxK	516.37	Joback Method
cpg	246.23	J/molxK	555.77	Joback Method
cpg	257.43	J/molxK	595.18	Joback Method
cpg	267.90	J/molxK	634.58	Joback Method
cpg	277.66	J/molxK	673.99	Joback Method
cpg	286.76	J/molxK	713.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4498991&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4498991&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>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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