

# 2-(Methylmercapto)benzonitrile

<b>Other names:</b>	2-(Methylthio)benzonitrile
<b>Inchi:</b>	InChI=1S/C8H7NS/c1-10-8-5-3-2-4-7(8)6-9/h2-5H,1H3
<b>InchiKey:</b>	PXZSANDJGNKIIA-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NS
<b>SMILES:</b>	CSc1cccc1C#N
<b>Mol. weight [g/mol]:</b>	149.21
<b>CAS:</b>	6609-54-7

## Physical Properties

Property code	Value	Unit	Source
gf	285.56	kJ/mol	Joback Method
hf	223.36	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	53.64	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.280		Crippen Method
mcvol	117.550	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	584.96	K	Joback Method
tc	838.73	K	Joback Method
tf	318.25	K	Joback Method
vc	0.456	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.04	J/mol×K	584.96	Joback Method
cpg	253.25	J/mol×K	627.25	Joback Method
cpg	262.72	J/mol×K	669.55	Joback Method
cpg	271.47	J/mol×K	711.84	Joback Method
cpg	279.51	J/mol×K	754.14	Joback Method
cpg	286.88	J/mol×K	796.43	Joback Method
cpg	293.58	J/mol×K	838.73	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.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>
<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=C6609547&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6609547&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>h vap:</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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