

# C4H4N2O2S

<b>Inchi:</b>	InChI=1S/C4H4N2O2S/c5-1-3-9(7,8)4-2-6/h3-4H2
<b>InchiKey:</b>	NNVQUTWFTPKDBS-UHFFFAOYSA-N
<b>Formula:</b>	C4H4N2O2S
<b>SMILES:</b>	N#CCS(=O)(=O)CC#N
<b>Mol. weight [g/mol]:</b>	144.15
<b>CAS:</b>	37463-94-8

## Physical Properties

Property code	Value	Unit	Source
gf	-219.38	kJ/mol	Joback Method
hf	-249.48	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	-0.552		Crippen Method
mcvol	98.070	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
tb	542.86	K	Joback Method
tc	750.03	K	Joback Method
tf	303.38	K	Joback Method
vc	0.438	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.48	J/molxK	542.86	Joback Method
cpg	202.54	J/molxK	577.39	Joback Method
cpg	208.29	J/molxK	611.92	Joback Method
cpg	213.71	J/molxK	646.45	Joback Method
cpg	218.78	J/molxK	680.98	Joback Method
cpg	223.51	J/molxK	715.50	Joback Method
cpg	227.88	J/molxK	750.03	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=C37463948&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37463948&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>mccvol:</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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