

# Thiocyanic acid, methylene ester

<b>Other names:</b>	Methane, dithiocyanato- Methylene bis(thiocyanate) Methylene dithiocyanate Methylene thiocyanate Methylenedirhodanide Nalfloc N 206 Methylendirhodanid Methylenedirhodanid Proxel MB Methylendithiokyanat Methylene ester of thiocyanic acid Antiblu 3737 Busan 110 Dithiocyanatomethane N-948 Biocide Nalco D-1994 Slimicide MC Tolcide MBT NSC 40464 Thiocyanic acid, C,C'-methylene ester V 709
<b>Inchi:</b>	InChI=1S/C3H2N2S2/c4-1-6-3-7-2-5/h3H2
<b>InchiKey:</b>	JWZXKXIUSSIAMR-UHFFFAOYSA-N
<b>Formula:</b>	C3H2N2S2
<b>SMILES:</b>	N#CSCSC#N
<b>Mol. weight [g/mol]:</b>	130.19
<b>CAS:</b>	6317-18-6

## Physical Properties

Property code	Value	Unit	Source
gf	306.98	kJ/mol	Joback Method
hf	308.25	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.372		Crippen Method

mvol	88.590	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	609.76	K	Joback Method
tc	870.09	K	Joback Method
tf	322.35	K	Joback Method
vc	0.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.40	J/mol×K	609.76	Joback Method
cpg	158.71	J/mol×K	653.15	Joback Method
cpg	162.70	J/mol×K	696.54	Joback Method
cpg	166.36	J/mol×K	739.93	Joback Method
cpg	169.68	J/mol×K	783.32	Joback Method
cpg	172.62	J/mol×K	826.70	Joback Method
cpg	175.17	J/mol×K	870.09	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6317186&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6317186&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>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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