

# Methional

<b>Other names:</b>	Propanal, 3-(methylthio)- Propionaldehyde, 3-(methylthio)- «beta»-(Methylmercapto)propionaldehyde «beta»-(Methylthio)propionaldehyde 3-(Methylmercapto)propionaldehyde 3-(Methylthio)propionaldehyde 3-Methylthiopropional Methylmercaptopropionic aldehyde 3-(Methylthio)propanal 4-Thiapentanal UN 2785 3-(Methylthio)-propanal 3-Methylmercaptopropyl aldehyde NSC 15874 3-(methylthio)propanal (methional) 3-Methylthio-1-propanal 3-(methylsulfanyl)propanal 3-(methylthio)propionaldehyde (methional) 3-(methylthiol)propanal
<b>Inchi:</b>	InChI=1S/C4H8OS/c1-6-4-2-3-5/h3H,2,4H2,1H3
<b>InchiKey:</b>	CLUWOWRTHNNBBU-UHFFFAOYSA-N
<b>Formula:</b>	C4H8OS
<b>SMILES:</b>	CSCCC=O
<b>Mol. weight [g/mol]:</b>	104.17
<b>CAS:</b>	3268-49-3

## Physical Properties

Property code	Value	Unit	Source
gf	-83.60	kJ/mol	Joback Method
hf	-169.60	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.938		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	915.00		NIST Webbook

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ripol	1495.00		NIST Webbook
ripol	1463.00		NIST Webbook
tb	438.70	K	NIST Webbook
tc	607.86	K	Joback Method
tf	211.24	K	Joback Method
vc	0.331	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.29	J/mol×K	408.36	Joback Method
cpg	158.00	J/mol×K	441.61	Joback Method
cpg	165.40	J/mol×K	474.86	Joback Method
cpg	172.50	J/mol×K	508.11	Joback Method
cpg	179.29	J/mol×K	541.36	Joback Method
cpg	185.79	J/mol×K	574.61	Joback Method
cpg	191.99	J/mol×K	607.86	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=C3268493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3268493&amp;Units=SI</a>
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<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>hvac:</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>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	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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