

# Methoxycarbonylsulfenyl chloride

<b>Other names:</b>	Carbonothioic acid, anhydrosulfide with thiohypochlorous acid, methyl ester thiocarbonic acid, anhydrosulphide with methyl thiohypochlorite
<b>Inchi:</b>	InChI=1S/C2H3ClO2S/c1-5-2(4)6-3/h1H3
<b>InchiKey:</b>	TXJXPZVVSLAQOQ-UHFFFAOYSA-N
<b>Formula:</b>	C2H3ClO2S
<b>SMILES:</b>	COC(=O)SCI
<b>Mol. weight [g/mol]:</b>	126.56
<b>CAS:</b>	26555-40-8

## Physical Properties

Property code	Value	Unit	Source
gf	-246.77	kJ/mol	Joback Method
hf	-303.28	kJ/mol	Joback Method
hfus	12.05	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.640		Crippen Method
mvol	75.070	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
tb	427.66	K	Joback Method
tc	644.29	K	Joback Method
tf	248.78	K	Joback Method
vc	0.275	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.15	J/molxK	427.66	Joback Method
cpg	121.47	J/molxK	463.77	Joback Method
cpg	125.70	J/molxK	499.87	Joback Method
cpg	129.84	J/molxK	535.98	Joback Method
cpg	133.84	J/molxK	572.08	Joback Method
cpg	137.70	J/molxK	608.19	Joback Method
cpg	141.40	J/molxK	644.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26555408&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26555408&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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