

# Bis(2-chloroethylthio)methane

<b>Inchi:</b>	InChI=1S/C5H10Cl2S2/c6-1-3-8-5-9-4-2-7/h1-5H2
<b>InchiKey:</b>	RKTJTAEKCRXNL-UHFFFAOYSA-N
<b>Formula:</b>	C5H10Cl2S2
<b>SMILES:</b>	CICCCSCCCCI
<b>Mol. weight [g/mol]:</b>	205.17
<b>CAS:</b>	63869-13-6

## Physical Properties

Property code	Value	Unit	Source
gf	33.60	kJ/mol	Joback Method
hf	-94.27	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.888		Crippen Method
mcvol	138.490	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	526.22	K	Joback Method
tc	752.80	K	Joback Method
tf	274.75	K	Joback Method
vc	0.521	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.39	J/molxK	526.22	Joback Method
cpg	270.34	J/molxK	563.98	Joback Method
cpg	279.76	J/molxK	601.75	Joback Method
cpg	288.64	J/molxK	639.51	Joback Method
cpg	296.98	J/molxK	677.27	Joback Method
cpg	304.79	J/molxK	715.03	Joback Method

## Sources

<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=C63869136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63869136&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>

## 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>rinpol:</b>	Non-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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