

# Bis(4-chlorophenylthio)methane

<b>Inchi:</b>	InChI=1S/C13H10Cl2S2/c14-10-1-5-12(6-2-10)16-9-17-13-7-3-11(15)4-8-13/h1-8H,9H2
<b>InchiKey:</b>	NTZBITFHYUVXFR-UHFFFAOYSA-N
<b>Formula:</b>	C13H10Cl2S2
<b>SMILES:</b>	Clc1ccc(SCSc2ccc(Cl)cc2)cc1
<b>Mol. weight [g/mol]:</b>	301.25
<b>CAS:</b>	2393-97-7

## Physical Properties

Property code	Value	Unit	Source
gf	306.52	kJ/mol	Joback Method
hf	190.73	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	72.81	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.835		Crippen Method
mcvol	203.690	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
tb	772.58	K	Joback Method
tc	1059.50	K	Joback Method
tf	442.79	K	Joback Method
vc	0.753	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.99	J/molxK	772.58	Joback Method
cpg	482.31	J/molxK	820.40	Joback Method
cpg	493.22	J/molxK	868.22	Joback Method
cpg	502.80	J/molxK	916.04	Joback Method
cpg	511.12	J/molxK	963.86	Joback Method
cpg	518.23	J/molxK	1011.68	Joback Method
cpg	524.23	J/molxK	1059.50	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C2393977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2393977&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>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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