

# Methyl 3-(4-chlorophenylthio)-2-methylpropionate

Inchi:	InChI=1S/C11H13ClO2S/c1-8(11(13)14-2)7-15-10-5-3-9(12)4-6-10/h3-6,8H,7H2,1-2H3
InchiKey:	LQTPIEYMBJPFQS-UHFFFAOYSA-N
Formula:	C11H13ClO2S
SMILES:	COC(=O)C(C)CSc1ccc(Cl)cc1
Mol. weight [g/mol]:	244.74
CAS:	55009-84-2

## Physical Properties

Property code	Value	Unit	Source
gf	-70.65	kJ/mol	Joback Method
hf	-269.26	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	62.99	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.241		Crippen Method
mvol	178.120	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	664.80	K	Joback Method
tc	900.59	K	Joback Method
tf	374.15	K	Joback Method
vc	0.664	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.82	J/molxK	664.80	Joback Method
cpg	437.25	J/molxK	704.10	Joback Method
cpg	449.70	J/molxK	743.40	Joback Method
cpg	461.20	J/molxK	782.70	Joback Method
cpg	471.76	J/molxK	821.99	Joback Method
cpg	481.40	J/molxK	861.29	Joback Method
cpg	490.12	J/molxK	900.59	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=C55009842&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55009842&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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