

# 3,4-Dichlorophenyl methanesulfonate

<b>Inchi:</b>	InChI=1S/C7H6Cl2O3S/c1-13(10,11)12-5-2-3-6(8)7(9)4-5/h2-4H,1H3
<b>InchiKey:</b>	VSSFDMFYXPXHKHF-UHFFFAOYSA-N
<b>Formula:</b>	C7H6Cl2O3S
<b>SMILES:</b>	CS(=O)(=O)Oc1ccc(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	241.09
<b>CAS:</b>	116401-62-8

## Physical Properties

Property code	Value	Unit	Source
gf	-496.19	kJ/mol	Joback Method
hf	-591.27	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	64.59	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.332		Crippen Method
mcvol	144.170	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	541.26	K	Joback Method
tc	759.41	K	Joback Method
tf	340.74	K	Joback Method
vc	0.561	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.02	J/molxK	541.26	Joback Method
cpg	288.97	J/molxK	577.62	Joback Method
cpg	298.36	J/molxK	613.98	Joback Method
cpg	307.18	J/molxK	650.34	Joback Method
cpg	315.43	J/molxK	686.69	Joback Method
cpg	323.07	J/molxK	723.05	Joback Method
cpg	330.11	J/molxK	759.41	Joback Method

# Sources

<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=C116401628&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401628&amp;Units=SI</a>
<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>

# 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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