

# 3,4-Dichlorophenyl isothiocyanate

<b>Other names:</b>	Benzene, 1,2-dichloro-4-isothiocyanato- Isothiocyanic acid, 3,4-dichlorophenyl ester 1,2-dichloro-4-isothiocyanatobenzene
<b>Inchi:</b>	InChI=1S/C7H3Cl2NS/c8-6-2-1-5(10-4-11)3-7(6)9/h1-3H
<b>InchiKey:</b>	OSBIEFWIIINTNJ-UHFFFAOYSA-N
<b>Formula:</b>	C7H3Cl2NS
<b>SMILES:</b>	S=C=Nc1ccc(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	204.08
<b>CAS:</b>	6590-94-9

## Physical Properties

Property code	Value	Unit	Source
hf	278.37	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.728		Crippen Method
mcvol	127.940	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	617.01	K	Joback Method
tc	892.29	K	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=C6590949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6590949&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>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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

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