

# Mycotox

<b>Other names:</b>	Phenol, 2,4,5-trichloro-, acetate Seedox Seedox 50 2,4,5-Trichlorophenol acetate 2,4,5-Trichlorophenyl acetate
<b>Inchi:</b>	InChI=1S/C8H5Cl3O2/c1-4(12)13-8-3-6(10)5(9)2-7(8)11/h2-3H,1H3
<b>InchiKey:</b>	IRMIPIZHLIHQST-UHFFFAOYSA-N
<b>Formula:</b>	C8H5Cl3O2
<b>SMILES:</b>	CC(=O)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	239.48
<b>CAS:</b>	5393-75-9

## Physical Properties

Property code	Value	Unit	Source
gf	-169.71	kJ/mol	Joback Method
hf	-298.35	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.572		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1511.00		NIST Webbook
ripol	2133.00		NIST Webbook
tb	612.64	K	Joback Method
tc	848.96	K	Joback Method
tf	405.82	K	Joback Method
vc	0.546	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	277.62	J/molxK	612.64	Joback Method
cpg	286.07	J/molxK	652.03	Joback Method
cpg	293.97	J/molxK	691.41	Joback Method
cpg	301.31	J/molxK	730.80	Joback Method
cpg	308.11	J/molxK	770.19	Joback Method
cpg	314.35	J/molxK	809.58	Joback Method
cpg	320.04	J/molxK	848.96	Joback Method
dvisc	0.0010302	Paxs	405.82	Joback Method
dvisc	0.0007244	Paxs	440.29	Joback Method
dvisc	0.0005361	Paxs	474.76	Joback Method
dvisc	0.0004132	Paxs	509.23	Joback Method
dvisc	0.0003292	Paxs	543.70	Joback Method
dvisc	0.0002695	Paxs	578.17	Joback Method
dvisc	0.0002256	Paxs	612.64	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5393759&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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