

# Phenol, 2,4-dichloro-, acetate

<b>Other names:</b>	2,4-Dichlorophenol acetate 2,4-Dichlorophenyl acetate Acetic acid, 2,4-dichlorophenyl ester
<b>Inchi:</b>	InChI=1S/C8H6Cl2O2/c1-5(11)12-8-3-2-6(9)4-7(8)10/h2-4H,1H3
<b>InchiKey:</b>	KGXUYVOKSRCTEK-UHFFFAOYSA-N
<b>Formula:</b>	C8H6Cl2O2
<b>SMILES:</b>	CC(=O)Oc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	205.04
<b>CAS:</b>	6341-97-5

## Physical Properties

Property code	Value	Unit	Source
gf	-148.15	kJ/mol	Joback Method
hf	-271.14	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
ie	8.16 ± 0.03	eV	NIST Webbook
log10ws	-3.16		Crippen Method
logp	2.919		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1351.00		NIST Webbook
ripol	1986.00		NIST Webbook
tb	517.70	K	NIST Webbook
tc	801.88	K	Joback Method
tf	363.38	K	Joback Method
vc	0.497	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/molxK	570.23	Joback Method
cpg	267.98	J/molxK	608.84	Joback Method
cpg	276.81	J/molxK	647.45	Joback Method
cpg	285.07	J/molxK	686.06	Joback Method
cpg	292.76	J/molxK	724.66	Joback Method
cpg	299.89	J/molxK	763.27	Joback Method
cpg	306.45	J/molxK	801.88	Joback Method
dvisc	0.0013093	Paxs	363.38	Joback Method
dvisc	0.0008718	Paxs	397.86	Joback Method
dvisc	0.0006194	Paxs	432.33	Joback Method
dvisc	0.0004628	Paxs	466.81	Joback Method
dvisc	0.0003600	Paxs	501.28	Joback Method
dvisc	0.0002892	Paxs	535.75	Joback Method
dvisc	0.0002386	Paxs	570.23	Joback Method

## Sources

<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=C6341975&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6341975&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## 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>ie:</b>	Ionization energy
<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
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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