

# Chloroacetic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C8H3Cl5O2/c9-2-5(14)15-8-4(11)1-3(10)6(12)7(8)13/h1H,2H2
InchiKey:	FTYKGQSYRRJQMV-UHFFFAOYSA-N
Formula:	C8H3Cl5O2
SMILES:	O=C(CCl)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	308.37

## Physical Properties

Property code	Value	Unit	Source
gf	-203.20	kJ/mol	Joback Method
hf	-341.30	kJ/mol	Joback Method
hfus	32.73	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.444		Crippen Method
mcvol	168.460	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1899.00		NIST Webbook
tb	692.48	K	Joback Method
tc	935.41	K	Joback Method
tf	478.18	K	Joback Method
vc	0.644	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.75	J/molxK	692.48	Joback Method
cpg	319.50	J/molxK	732.97	Joback Method
cpg	325.72	J/molxK	773.46	Joback Method
cpg	331.38	J/molxK	813.94	Joback Method
cpg	336.49	J/molxK	854.43	Joback Method
cpg	341.04	J/molxK	894.92	Joback Method
cpg	345.04	J/molxK	935.41	Joback Method
dvisc	0.0007537	Paxs	478.18	Joback Method
dvisc	0.0005541	Paxs	513.90	Joback Method

dvisc	0.0004239	Paxs	549.61	Joback Method
dvisc	0.0003351	Paxs	585.33	Joback Method
dvisc	0.0002722	Paxs	621.05	Joback Method
dvisc	0.0002261	Paxs	656.76	Joback Method
dvisc	0.0001915	Paxs	692.48	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=U354614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354614&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>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>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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