

# Dibenzo-p-dioxin, 1,2,3-trichloro

<b>Inchi:</b>	InChI=1S/C12H5Cl3O2/c13-6-5-9-12(11(15)10(6)14)17-8-4-2-1-3-7(8)16-9/h1-5H
<b>InchiKey:</b>	SKMFBGZVVNDVFR-UHFFFAOYSA-N
<b>Formula:</b>	C12H5Cl3O2
<b>SMILES:</b>	Clc1cc2c(c(Cl)c1Cl)Oc1ccccc1O2
<b>Mol. weight [g/mol]:</b>	287.53

## Physical Properties

Property code	Value	Unit	Source
gf	99.36	kJ/mol	Joback Method
hf	-87.22	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	5.545		Crippen Method
mcvol	170.020	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	725.55	K	Joback Method
tc	990.47	K	Joback Method
tf	509.04	K	Joback Method
vc	0.646	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.96	J/molxK	725.55	Joback Method
cpg	383.94	J/molxK	769.70	Joback Method
cpg	392.18	J/molxK	813.86	Joback Method
cpg	399.78	J/molxK	858.01	Joback Method
cpg	406.87	J/molxK	902.16	Joback Method
cpg	413.56	J/molxK	946.32	Joback Method
cpg	419.96	J/molxK	990.47	Joback Method

dvisc	0.0013574	Paxs	509.04	Joback Method
dvisc	0.0010829	Paxs	545.13	Joback Method
dvisc	0.0008885	Paxs	581.21	Joback Method
dvisc	0.0007461	Paxs	617.30	Joback Method
dvisc	0.0006387	Paxs	653.38	Joback Method
dvisc	0.0005557	Paxs	689.47	Joback Method
dvisc	0.0004903	Paxs	725.55	Joback Method

## Sources

<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>
<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=R50127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R50127&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>mvol:</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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