

# 1,4,7,8-tetrachloro dibenzo-p-dioxin

<b>Other names:</b>	Dibenzo-p-dioxin, 1,4,7,8-tetrachloro 1,4,7,8-tetrachlorodibenzodioxin
<b>Inchi:</b>	InChI=1S/C12H4Cl4O2/c13-5-1-2-6(14)12-11(5)17-9-3-7(15)8(16)4-10(9)18-12/h1-4H
<b>InchiKey:</b>	FCRXUTCUWCJZJI-UHFFFAOYSA-N
<b>Formula:</b>	C12H4Cl4O2
<b>SMILES:</b>	Clc1cc2c(cc1Cl)Oc1c(Cl)ccc(Cl)c1O2
<b>Mol. weight [g/mol]:</b>	321.97

## Physical Properties

Property code	Value	Unit	Source
gf	77.80	kJ/mol	Joback Method
hf	-114.43	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	6.198		Crippen Method
mcvol	182.260	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	767.96	K	Joback Method
tc	1035.13	K	Joback Method
tf	551.48	K	Joback Method
vc	0.696	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	390.63	J/molxK	767.96	Joback Method
cpg	425.28	J/molxK	990.60	Joback Method
cpg	419.14	J/molxK	946.08	Joback Method
cpg	412.71	J/molxK	901.55	Joback Method
cpg	405.89	J/molxK	857.02	Joback Method
cpg	398.57	J/molxK	812.49	Joback Method
cpg	431.25	J/molxK	1035.13	Joback Method
dvisc	0.0004605	Paxs	767.96	Joback Method
dvisc	0.0005188	Paxs	731.88	Joback Method
dvisc	0.0005917	Paxs	695.80	Joback Method
dvisc	0.0006847	Paxs	659.72	Joback Method
dvisc	0.0008058	Paxs	623.64	Joback Method
dvisc	0.0009675	Paxs	587.56	Joback Method
dvisc	0.0011898	Paxs	551.48	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=R37638&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R37638&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>

## 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>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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