

# 1,3,7,9-tetrabromo-2,8-dichloro-dibenzo-p-dioxin

<b>Other names:</b>	Dibenzodioxin, 1,3,7,9-tetrabromo-, 2,8-dichloro-
<b>Inchi:</b>	InChI=1S/C12H2Br4Cl2O2/c13-3-1-5-11(7(15)9(3)17)20-12-6(19-5)2-4(14)10(18)8(12)16
<b>InchiKey:</b>	KEJDZQDFLNGFOO-UHFFFAOYSA-N
<b>Formula:</b>	C12H2Br4Cl2O2
<b>SMILES:</b>	Clc1c(Br)cc2c(c1Br)Oc1c(cc(Br)c(Cl)c1Br)O2
<b>Mol. weight [g/mol]:</b>	568.66

## Physical Properties

Property code	Value	Unit	Source
gf	139.68	kJ/mol	Joback Method
hf	-0.57	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.941		Crippen Method
mcpvol	227.780	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	967.70	K	Joback Method
tc	1266.25	K	Joback Method
tf	755.88	K	Joback Method
vc	0.846	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.76	J/molxK	967.70	Joback Method
cpg	475.92	J/molxK	1216.49	Joback Method
cpg	466.35	J/molxK	1166.73	Joback Method
cpg	457.76	J/molxK	1116.97	Joback Method
cpg	449.93	J/molxK	1067.22	Joback Method
cpg	442.66	J/molxK	1017.46	Joback Method

cpg	486.67	J/mol×K	1266.25	Joback Method
dvisc	0.0002767	Paxs	967.70	Joback Method
dvisc	0.0003058	Paxs	932.40	Joback Method
dvisc	0.0003405	Paxs	897.09	Joback Method
dvisc	0.0003826	Paxs	861.79	Joback Method
dvisc	0.0004342	Paxs	826.49	Joback Method
dvisc	0.0004983	Paxs	791.18	Joback Method
dvisc	0.0005793	Paxs	755.88	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=R171212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R171212&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>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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