

# 2,9-dibromo,1,3-dichloro-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12H4Br2Cl2O2/c13-5-2-1-3-7-11(5)18-12-8(17-7)4-6(15)9(14)10(12)16/h1-4H
<b>InchiKey:</b>	ILSNBLBXR DOPFR-UHFFFAOYSA-N
<b>Formula:</b>	C12H4Br2Cl2O2
<b>SMILES:</b>	Clc1cc2c(c(Cl)c1Br)Oc1c(Br)cccc1O2
<b>Mol. weight [g/mol]:</b>	410.87

## Physical Properties

Property code	Value	Unit	Source
gf	130.30	kJ/mol	Joback Method
hf	-30.29	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	81.54	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.416		Crippen Method
mcvol	192.780	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinsol	2587.00		NIST Webbook
tb	825.42	K	Joback Method
tc	1108.05	K	Joback Method
tf	611.24	K	Joback Method
vc	0.722	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.92	J/molxK	825.42	Joback Method
cpg	437.04	J/molxK	1060.95	Joback Method
cpg	430.15	J/molxK	1013.84	Joback Method
cpg	423.35	J/molxK	966.74	Joback Method
cpg	416.49	J/molxK	919.63	Joback Method
cpg	409.40	J/molxK	872.53	Joback Method
cpg	444.20	J/molxK	1108.05	Joback Method
dvisc	0.0004177	Paxs	825.42	Joback Method
dvisc	0.0004681	Paxs	789.72	Joback Method

dvisc	0.0005304	Paxs	754.03	Joback Method
dvisc	0.0006085	Paxs	718.33	Joback Method
dvisc	0.0007082	Paxs	682.63	Joback Method
dvisc	0.0008382	Paxs	646.94	Joback Method
dvisc	0.0010117	Paxs	611.24	Joback Method

## Sources

<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>
<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=R172760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172760&amp;Units=SI</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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