

# Dibenzodioxin, 1,4,9-tribromo-, 2,7-dichloro-

<b>Other names:</b>	1,4,9-tribromo-2,7-dichlorodibenzo-p-dioxin
<b>Inchi:</b>	InChI=1S/C12H3Br3Cl2O2/c13-5-1-4(16)2-8-10(5)19-12-9(15)7(17)3-6(14)11(12)18-8/h1
<b>InchiKey:</b>	DFIVEIMXCWUCRB-UHFFFAOYSA-N
<b>Formula:</b>	C12H3Br3Cl2O2
<b>SMILES:</b>	Clc1cc(Br)c2c(c1)Oc1c(Br)cc(Cl)c(Br)c1O2
<b>Mol. weight [g/mol]:</b>	489.77

## Physical Properties

Property code	Value	Unit	Source
gf	134.99	kJ/mol	Joback Method
hf	-15.43	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.179		Crippen Method
mcpvol	210.280	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	896.56	K	Joback Method
tc	1187.57	K	Joback Method
tf	683.56	K	Joback Method
vc	0.783	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.58	J/molxK	896.56	Joback Method
cpg	426.45	J/molxK	945.06	Joback Method
cpg	433.27	J/molxK	993.56	Joback Method
cpg	440.23	J/molxK	1042.06	Joback Method
cpg	447.51	J/molxK	1090.57	Joback Method
cpg	455.30	J/molxK	1139.07	Joback Method

cpg	463.77	J/molxK	1187.57	Joback Method
dvisc	0.0007743	Paxs	683.56	Joback Method
dvisc	0.0006549	Paxs	719.06	Joback Method
dvisc	0.0005628	Paxs	754.56	Joback Method
dvisc	0.0004902	Paxs	790.06	Joback Method
dvisc	0.0004321	Paxs	825.56	Joback Method
dvisc	0.0003849	Paxs	861.06	Joback Method
dvisc	0.0003460	Paxs	896.56	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=R171396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R171396&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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