

# Dibenzodioxin, 3,8-dibromo-, 1,2,6,7-tetrachloro-

<b>Inchi:</b>	InChI=1S/C12H2Br3Cl3O2/c13-3-1-5-11(7(15)8(3)16)19-6-2-4(14)9(17)10(18)12(6)20-5/
<b>InchiKey:</b>	SLXSNXPRNVONFS-UHFFFAOYSA-N
<b>Formula:</b>	C12H2Br3Cl3O2
<b>SMILES:</b>	Clc1c(Br)cc2c(c1Cl)Oc1cc(Br)c(Cl)c(Br)c1O2
<b>Mol. weight [g/mol]:</b>	524.21

## Physical Properties

Property code	Value	Unit	Source
gf	113.43	kJ/mol	Joback Method
hf	-42.64	kJ/mol	Joback Method
hfus	55.37	kJ/mol	Joback Method
hvap	93.68	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.832		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinqol	2990.00		NIST Webbook
tb	938.97	K	Joback Method
tc	1230.73	K	Joback Method
tf	726.00	K	Joback Method
vc	0.833	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.25	J/molxK	938.97	Joback Method
cpg	437.74	J/molxK	987.60	Joback Method
cpg	444.35	J/molxK	1036.22	Joback Method
cpg	451.24	J/molxK	1084.85	Joback Method
cpg	458.59	J/molxK	1133.48	Joback Method
cpg	466.58	J/molxK	1182.11	Joback Method
cpg	475.38	J/molxK	1230.73	Joback Method
dvisc	0.0006566	Paxs	726.00	Joback Method
dvisc	0.0005615	Paxs	761.50	Joback Method

dvisc	0.0004869	Paxs	796.99	Joback Method
dvisc	0.0004273	Paxs	832.49	Joback Method
dvisc	0.0003791	Paxs	867.98	Joback Method
dvisc	0.0003395	Paxs	903.48	Joback Method
dvisc	0.0003066	Paxs	938.97	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R317512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R317512&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.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>

## 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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