

# Dibenzodioxin, 1,9-dibromo-, 2,3,7,8-tetrachloro-

Inchi:	InChI=1S/C12H2Br2Cl4O2/c13-7-9(17)3(15)1-5-11(7)20-12-6(19-5)2-4(16)10(18)8(12)14
InchiKey:	SKYSVRMBQVOVEL-UHFFFAOYSA-N
Formula:	C12H2Br2Cl4O2
SMILES:	Clc1cc2c(c(Br)c1Cl)Oc1c(cc(Cl)c(Cl)c1Br)O2
Mol. weight [g/mol]:	479.76

## Physical Properties

Property code	Value	Unit	Source
gf	87.18	kJ/mol	Joback Method
hf	-84.71	kJ/mol	Joback Method
hfus	54.29	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.723		Crippen Method
mcvol	217.260	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinqol	2994.00		NIST Webbook
tb	910.24	K	Joback Method
tc	1195.12	K	Joback Method
tf	696.12	K	Joback Method
vc	0.820	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.85	J/molxK	910.24	Joback Method
cpg	433.11	J/molxK	957.72	Joback Method
cpg	439.29	J/molxK	1005.20	Joback Method
cpg	445.52	J/molxK	1052.68	Joback Method
cpg	451.96	J/molxK	1100.16	Joback Method
cpg	458.74	J/molxK	1147.64	Joback Method
cpg	466.02	J/molxK	1195.12	Joback Method
dvisc	0.0007377	Paxs	696.12	Joback Method
dvisc	0.0006269	Paxs	731.81	Joback Method

dvisc	0.0005408	Paxs	767.49	Joback Method
dvisc	0.0004727	Paxs	803.18	Joback Method
dvisc	0.0004180	Paxs	838.87	Joback Method
dvisc	0.0003733	Paxs	874.55	Joback Method
dvisc	0.0003364	Paxs	910.24	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=R317116&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R317116&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>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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