

# 1-bromo,2,3,6-trichloro-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12H4BrCl3O2/c13-9-10(16)6(15)4-8-12(9)17-7-3-1-2-5(14)11(7)18-8/h1-4H
<b>InchiKey:</b>	ANMFZXIBGVXYQJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H4BrCl3O2
<b>SMILES:</b>	Clc1cc2c(c(Br)c1Cl)Oc1cccc(Cl)c1O2
<b>Mol. weight [g/mol]:</b>	366.42

## Physical Properties

Property code	Value	Unit	Source
gf	104.05	kJ/mol	Joback Method
hf	-72.36	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.307		Crippen Method
mcvol	187.520	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	796.69	K	Joback Method
tc	1071.66	K	Joback Method
tf	581.36	K	Joback Method
vc	0.709	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.46	J/molxK	796.69	Joback Method
cpg	430.95	J/molxK	1025.83	Joback Method
cpg	424.55	J/molxK	980.00	Joback Method
cpg	418.04	J/molxK	934.17	Joback Method
cpg	411.28	J/molxK	888.35	Joback Method
cpg	404.13	J/molxK	842.52	Joback Method
cpg	437.37	J/molxK	1071.66	Joback Method
dvisc	0.0004427	Paxs	796.69	Joback Method

dvisc	0.0004974	Paxs	760.80	Joback Method
dvisc	0.0005655	Paxs	724.91	Joback Method
dvisc	0.0006515	Paxs	689.03	Joback Method
dvisc	0.0007624	Paxs	653.14	Joback Method
dvisc	0.0009086	Paxs	617.25	Joback Method
dvisc	0.0011065	Paxs	581.36	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=R172631&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172631&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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