

# 2,3,7-tribromo,8-chloro-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12H4Br3ClO2/c13-5-1-9-10(2-6(5)14)18-12-4-8(16)7(15)3-11(12)17-9/h1-4H
<b>InchiKey:</b>	VAPXVPBAPGEGAW-UHFFFAOYSA-N
<b>Formula:</b>	C12H4Br3ClO2
<b>SMILES:</b>	Clc1cc2c(cc1Br)Oc1cc(Br)c(Br)cc1O2
<b>Mol. weight [g/mol]:</b>	455.32

## Physical Properties

Property code	Value	Unit	Source
gf	156.55	kJ/mol	Joback Method
hf	11.78	kJ/mol	Joback Method
hfus	47.76	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.526		Crippen Method
mcvol	198.040	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinsol	2702.00		NIST Webbook
tb	854.15	K	Joback Method
tc	1144.33	K	Joback Method
tf	641.12	K	Joback Method
vc	0.735	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/molxK	854.15	Joback Method
cpg	414.50	J/molxK	902.51	Joback Method
cpg	421.68	J/molxK	950.88	Joback Method
cpg	428.84	J/molxK	999.24	Joback Method
cpg	436.15	J/molxK	1047.60	Joback Method
cpg	443.83	J/molxK	1095.96	Joback Method
cpg	452.05	J/molxK	1144.33	Joback Method
dvisc	0.0009125	Paxs	641.12	Joback Method
dvisc	0.0007623	Paxs	676.62	Joback Method

dvisc	0.0006483	Paxs	712.13	Joback Method
dvisc	0.0005599	Paxs	747.63	Joback Method
dvisc	0.0004901	Paxs	783.14	Joback Method
dvisc	0.0004339	Paxs	818.64	Joback Method
dvisc	0.0003881	Paxs	854.15	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R172715&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172715&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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