

# 1,2-dibromo-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12H6Br2O2/c13-7-5-6-10-12(11(7)14)16-9-4-2-1-3-8(9)15-10/h1-6H
<b>InchiKey:</b>	MKXZILBIAQNODC-UHFFFAOYSA-N
<b>Formula:</b>	C12H6Br2O2
<b>SMILES:</b>	BrC1ccc2c(c1Br)Oc1ccccc1O2
<b>Mol. weight [g/mol]:</b>	341.98

## Physical Properties

Property code	Value	Unit	Source
gf	173.42	kJ/mol	Joback Method
hf	24.13	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.110		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	740.60	K	Joback Method
tc	1020.08	K	Joback Method
tf	526.36	K	Joback Method
vc	0.624	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.39	J/molxK	740.60	Joback Method
cpg	413.49	J/molxK	973.50	Joback Method
cpg	406.06	J/molxK	926.92	Joback Method
cpg	398.41	J/molxK	880.34	Joback Method
cpg	390.37	J/molxK	833.76	Joback Method
cpg	381.75	J/molxK	787.18	Joback Method
cpg	420.88	J/molxK	1020.08	Joback Method
dvisc	0.0005007	Paxs	740.60	Joback Method

dvisc	0.0005680	Paxs	704.89	Joback Method
dvisc	0.0006531	Paxs	669.19	Joback Method
dvisc	0.0007629	Paxs	633.48	Joback Method
dvisc	0.0009077	Paxs	597.77	Joback Method
dvisc	0.0011043	Paxs	562.07	Joback Method
dvisc	0.0013795	Paxs	526.36	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=R172453&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172453&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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