

# 1-bromo,2,3,4,6,7,9-hexachloro-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12HBrCl6O2/c13-4-6(17)7(18)8(19)12-10(4)20-9-3(15)1-2(14)5(16)11(9)21-1
<b>InchiKey:</b>	SULWTINSLHJMIT-UHFFFAOYSA-N
<b>Formula:</b>	C12HBrCl6O2
<b>SMILES:</b>	Clc1cc(Cl)c2c(c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Br)c1O2
<b>Mol. weight [g/mol]:</b>	469.76

## Physical Properties

Property code	Value	Unit	Source
gf	39.37	kJ/mol	Joback Method
hf	-153.99	kJ/mol	Joback Method
hfus	57.01	kJ/mol	Joback Method
hvap	94.63	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	8.268		Crippen Method
mcvol	224.240	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	923.92	K	Joback Method
tc	1203.14	K	Joback Method
tf	708.68	K	Joback Method
vc	0.856	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.87	J/mol×K	923.92	Joback Method
cpg	461.87	J/mol×K	1156.61	Joback Method
cpg	456.10	J/mol×K	1110.07	Joback Method
cpg	450.53	J/mol×K	1063.53	Joback Method
cpg	445.05	J/mol×K	1016.99	Joback Method
cpg	439.53	J/mol×K	970.46	Joback Method
cpg	467.95	J/mol×K	1203.14	Joback Method
dvisc	0.0003272	Paxs	923.92	Joback Method

dvisc	0.0003623	Paxs	888.05	Joback Method
dvisc	0.0004046	Paxs	852.17	Joback Method
dvisc	0.0004562	Paxs	816.30	Joback Method
dvisc	0.0005202	Paxs	780.43	Joback Method
dvisc	0.0006007	Paxs	744.55	Joback Method
dvisc	0.0007039	Paxs	708.68	Joback Method

## Sources

<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=R172611&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172611&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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