

# 1,2,3,4,6,7-hexabromo-dibenzo-dioxin

<b>Inchi:</b>	InChI=1S/C12H2Br6O2/c13-3-1-2-4-10(5(3)14)20-12-9(18)7(16)6(15)8(17)11(12)19-4/h1
<b>InchiKey:</b>	RZDHYIJHBJEYLW-UHFFFAOYSA-N
<b>Formula:</b>	C12H2Br6O2
<b>SMILES:</b>	BrC1ccc2c(c1Br)Oc1c(Br)c(Br)c(Br)c(Br)c1O2
<b>Mol. weight [g/mol]:</b>	657.57

## Physical Properties

Property code	Value	Unit	Source
gf	192.18	kJ/mol	Joback Method
hf	83.57	kJ/mol	Joback Method
hfus	58.64	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	8.160		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
rinpol	3579.00		NIST Webbook
rinpol	3579.00		NIST Webbook
tb	1025.16	K	Joback Method
tc	1336.99	K	Joback Method
tf	815.64	K	Joback Method
vc	0.872	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.63	J/molxK	1025.16	Joback Method
cpg	454.07	J/molxK	1077.13	Joback Method
cpg	463.50	J/molxK	1129.10	Joback Method
cpg	474.20	J/molxK	1181.08	Joback Method
cpg	486.42	J/molxK	1233.05	Joback Method
cpg	500.46	J/molxK	1285.02	Joback Method
cpg	516.60	J/molxK	1336.99	Joback Method
dvisc	0.0004414	Paxs	815.64	Joback Method

dvisc	0.0003838	Paxs	850.56	Joback Method
dvisc	0.0003374	Paxs	885.48	Joback Method
dvisc	0.0002996	Paxs	920.40	Joback Method
dvisc	0.0002683	Paxs	955.32	Joback Method
dvisc	0.0002421	Paxs	990.24	Joback Method
dvisc	0.0002201	Paxs	1025.16	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R172324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172324&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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