

# Benzo[b]benzo[3,4]cyclobuta[1,2-e][1,4]dioxin,

Other names:

3,4,7,8-Dibenzo-2,5-dioxabicyclo[4.2.0]octa-3,7-diene

**4b,10a-dihydro-**

InChI=1S/C14H10O2/c1-2-6-10-9(5-1)13-14(10)16-12-8-4-3-7-11(12)15-13/h1-8,13-14H

**InchiKey:** SSPWYTLOLFHBPK-UHFFFAOYSA-N

**Formula:** C14H10O2

**SMILES:** c1ccc2c(c1)OC1c3ccccc3C1O2

**Mol. weight [g/mol]:** 210.23

**CAS:** 42896-18-4

## Physical Properties

Property code	Value	Unit	Source
gf	246.02	kJ/mol	Joback Method
hf	11.75	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
ie	7.60 ± 0.02	eV	NIST Webbook
log10ws	-4.00		Crippen Method
logp	3.254		Crippen Method
mcvol	150.620	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	641.88	K	Joback Method
tc	895.06	K	Joback Method
tf	421.48	K	Joback Method
vc	0.576	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.48	J/molxK	641.88	Joback Method
cpg	412.96	J/molxK	684.08	Joback Method
cpg	426.17	J/molxK	726.27	Joback Method
cpg	438.29	J/molxK	768.47	Joback Method
cpg	449.51	J/molxK	810.66	Joback Method
cpg	459.99	J/molxK	852.86	Joback Method
cpg	469.93	J/molxK	895.06	Joback Method

dvisc	0.0029382	Paxs	421.48	Joback Method
dvisc	0.0026272	Paxs	458.21	Joback Method
dvisc	0.0023884	Paxs	494.95	Joback Method
dvisc	0.0022001	Paxs	531.68	Joback Method
dvisc	0.0020483	Paxs	568.41	Joback Method
dvisc	0.0019235	Paxs	605.15	Joback Method
dvisc	0.0018194	Paxs	641.88	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=C42896184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42896184&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>ie:</b>	Ionization energy
<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>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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