

# Acetic acid, bromo(o-hydroxyphenyl)phenyl-, gamma-lactone

<b>Inchi:</b>	InChI=1S/C14H9BrO2/c15-14(10-6-2-1-3-7-10)11-8-4-5-9-12(11)17-13(14)16/h1-9H
<b>InchiKey:</b>	BFZJRNTVOKVQLW-UHFFFAOYSA-N
<b>Formula:</b>	C14H9BrO2
<b>SMILES:</b>	O=C1Oc2ccccc2C1(Br)c1cccc1
<b>Mol. weight [g/mol]:</b>	289.12
<b>CAS:</b>	51656-58-7

## Physical Properties

Property code	Value	Unit	Source
gf	143.06	kJ/mol	Joback Method
hf	-26.03	kJ/mol	Joback Method
hfus	24.32	kJ/mol	Joback Method
hvap	65.93	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.244		Crippen Method
mcvol	174.680	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
tb	745.97	K	Joback Method
tc	1035.14	K	Joback Method
tf	509.33	K	Joback Method
vc	0.648	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.05	J/molxK	745.97	Joback Method
cpg	457.46	J/molxK	794.17	Joback Method
cpg	471.27	J/molxK	842.36	Joback Method
cpg	484.81	J/molxK	890.56	Joback Method
cpg	498.41	J/molxK	938.75	Joback Method
cpg	512.40	J/molxK	986.95	Joback Method
cpg	527.11	J/molxK	1035.14	Joback Method

# Sources

<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=C51656587&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51656587&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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>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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