

# Benzene, 4-bromo-1,2-dimethoxy-

<b>Other names:</b>	1-Bromo-3,4-dimethoxybenzene 4-Bromo-1,2-dimethoxybenzene 4-Bromoveratrole 3,4-Dimethoxybromobenzene 3,4-Dimethoxyphenyl bromide p-Bromoveratrole 4-Bromoguaiacol, methyl ether Bromoveratrole
<b>Inchi:</b>	InChI=1S/C8H9BrO2/c1-10-7-4-3-6(9)5-8(7)11-2/h3-5H,1-2H3
<b>InchiKey:</b>	KBTMGSMZIKLAHN-UHFFFAOYSA-N
<b>Formula:</b>	C8H9BrO2
<b>SMILES:</b>	COc1ccc(Br)cc1OC
<b>Mol. weight [g/mol]:</b>	217.06
<b>CAS:</b>	2859-78-1

## Physical Properties

Property code	Value	Unit	Source
gf	-86.05	kJ/mol	Joback Method
hf	-232.97	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	48.26	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.466		Crippen Method
mcvol	129.060	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	1423.70		NIST Webbook
rinpol	1423.70		NIST Webbook
tb	528.70	K	NIST Webbook
tc	755.88	K	Joback Method
tf	335.64	K	Joback Method
vc	0.473	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.01	J/mol×K	530.08	Joback Method
cpg	266.93	J/mol×K	567.71	Joback Method
cpg	277.32	J/mol×K	605.35	Joback Method
cpg	287.19	J/mol×K	642.98	Joback Method
cpg	296.52	J/mol×K	680.61	Joback Method
cpg	305.31	J/mol×K	718.25	Joback Method
cpg	313.56	J/mol×K	755.88	Joback Method
dvisc	0.0010073	Paxs	335.64	Joback Method
dvisc	0.0006754	Paxs	368.05	Joback Method
dvisc	0.0004832	Paxs	400.45	Joback Method
dvisc	0.0003634	Paxs	432.86	Joback Method
dvisc	0.0002844	Paxs	465.27	Joback Method
dvisc	0.0002298	Paxs	497.67	Joback Method
dvisc	0.0001906	Paxs	530.08	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=C2859781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2859781&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>

## 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

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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