

# 1,2-Propadiene, 1-bromo-

<b>Other names:</b>	Propa-1,2-diene, 1-bromo- 1-Bromopropadiene
<b>Inchi:</b>	InChI=1S/C3H3Br/c1-2-3-4/h3H,1H2
<b>InchiKey:</b>	UUIORUQWCRSGJS-UHFFFAOYSA-N
<b>Formula:</b>	C3H3Br
<b>SMILES:</b>	C=C=CBr
<b>Mol. weight [g/mol]:</b>	118.96
<b>CAS:</b>	10024-18-7

## Physical Properties

Property code	Value	Unit	Source
gf	204.82	kJ/mol	Joback Method
hf	209.29	kJ/mol	Joback Method
hfus	9.66	kJ/mol	Joback Method
hvap	28.47	kJ/mol	Joback Method
ie	9.46	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.680		Crippen Method
mcvol	62.030	ml/mol	McGowan Method
pc	5889.94	kPa	Joback Method
tb	334.15	K	Joback Method
tc	538.01	K	Joback Method
tf	188.12	K	Joback Method
vc	0.227	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.67	J/mol×K	334.15	Joback Method
cpg	81.29	J/mol×K	368.13	Joback Method
cpg	84.76	J/mol×K	402.10	Joback Method
cpg	88.09	J/mol×K	436.08	Joback Method
cpg	91.28	J/mol×K	470.05	Joback Method
cpg	94.34	J/mol×K	504.03	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=C10024187&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10024187&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>h vap:</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>m cvol:</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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