

# 2-Butene, 1-bromo-

<b>Other names:</b>	1-Bromo-2-butene 1-Crotyl bromide 1-bromobut-2-ene 2-Butenyl bromide Crotonyl bromide Crotyl bromide
<b>Inchi:</b>	InChI=1S/C4H7Br/c1-2-3-4-5/h2-3H,4H2,1H3/b3-2+
<b>InchiKey:</b>	AVMHMVJVHYGDOO-NSCUHMNNSA-N
<b>Formula:</b>	C4H7Br
<b>SMILES:</b>	CC=CCBr
<b>Mol. weight [g/mol]:</b>	135.00
<b>CAS:</b>	4784-77-4

## Physical Properties

Property code	Value	Unit	Source
gf	77.34	kJ/mol	Joback Method
hf	17.66	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	30.89	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.957		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	371.15 ± 2.00	K	NIST Webbook
tb	377.50 ± 1.50	K	NIST Webbook
tc	557.14	K	Joback Method
tf	189.56	K	Joback Method
vc	0.301	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.95	J/mol×K	361.24	Joback Method
cpg	120.43	J/mol×K	393.89	Joback Method

cpg	127.45	J/molxK	426.54	Joback Method
cpg	134.06	J/molxK	459.19	Joback Method
cpg	140.27	J/molxK	491.84	Joback Method
cpg	146.10	J/molxK	524.49	Joback Method
cpg	151.59	J/molxK	557.14	Joback Method
dvisc	0.0032305	Paxs	189.56	Joback Method
dvisc	0.0016765	Paxs	218.17	Joback Method
dvisc	0.0010129	Paxs	246.79	Joback Method
dvisc	0.0006796	Paxs	275.40	Joback Method
dvisc	0.0004915	Paxs	304.01	Joback Method
dvisc	0.0003758	Paxs	332.63	Joback Method
dvisc	0.0002999	Paxs	361.24	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	286.00	K	1.30	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53332e+01
Coeff. B	-3.55050e+03
Coeff. C	-4.61370e+01
Temperature range (K), min.	282.12
Temperature range (K), max.	400.62

## Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4784774&Units=SI>

**The Yaws Handbook of Vapor Pressure:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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