

1-Butene, 4-bromo-

Other names:	1-Bromo-3-butene 3-Butenyl bromide 4-Bromo-1-butene 4-Bromobutene 4-Bromobutene-(1) 4-bromobut-1-ene Homoallyl bromide
Inchi:	InChI=1S/C4H7Br/c1-2-3-4-5/h2H,1,3-4H2
InchiKey:	DMAYBPBPEUFIHJ-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	C=CCCBBr
Mol. weight [g/mol]:	135.00
CAS:	5162-44-7

Physical Properties

Property code	Value	Unit	Source
gf	84.96	kJ/mol	Joback Method
hf	25.87	kJ/mol	Joback Method
hfus	10.12	kJ/mol	Joback Method
hvap	30.26	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.957		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
rinpol	695.00		NIST Webbook
tb	371.70	K	NIST Webbook
tb	371.60	K	NIST Webbook
tc	543.41	K	Joback Method
tf	192.88	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.50	J/mol×K	353.76	Joback Method
cpg	121.62	J/mol×K	385.37	Joback Method
cpg	128.36	J/mol×K	416.98	Joback Method
cpg	134.74	J/mol×K	448.59	Joback Method
cpg	140.79	J/mol×K	480.20	Joback Method
cpg	146.52	J/mol×K	511.81	Joback Method
cpg	151.93	J/mol×K	543.41	Joback Method
dvisc	0.0029889	Pa×s	192.88	Joback Method
dvisc	0.0016840	Pa×s	219.69	Joback Method
dvisc	0.0010749	Pa×s	246.51	Joback Method
dvisc	0.0007493	Pa×s	273.32	Joback Method
dvisc	0.0005571	Pa×s	300.13	Joback Method
dvisc	0.0004349	Pa×s	326.95	Joback Method
dvisc	0.0003524	Pa×s	353.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37847e+01
Coeff. B	-2.57474e+03
Coeff. C	-9.08090e+01
Temperature range (K), min.	281.57
Temperature range (K), max.	395.02

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

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

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5162447&Units=SI>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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