

1-Propene, 3-bromo-

Other names:	1-BROMO-2-PROPENE 2-PROPENYL BROMIDE 3-Bromo-1-propene 3-Bromopropene 3-Bromopropylene 3-bromoprop-1-ene ALLYL BROMIDE Bromallylene CH ₂ =CHCH ₂ Br NSC 7596 Propene, 3-bromo- UN 1099
Inchi:	InChI=1S/C3H5Br/c1-2-3-4/h2H,1,3H2
InchiKey:	BHELZAPQIKSEDF-UHFFFAOYSA-N
Formula:	C ₃ H ₅ Br
SMILES:	C=CCBr
Mol. weight [g/mol]:	120.98
CAS:	106-95-6

Physical Properties

Property code	Value	Unit	Source
af	0.2730		KDB
gf	76.54	kJ/mol	Joback Method
hf	45.60 ± 6.70	kJ/mol	NIST Webbook
hf	47.70	kJ/mol	NIST Webbook
hfl	20.00	kJ/mol	NIST Webbook
hfl	13.00 ± 5.90	kJ/mol	NIST Webbook
hfus	7.53	kJ/mol	Joback Method
hvap	32.85	kJ/mol	NIST Webbook
hvap	33.00 ± 2.00	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	9.96	eV	NIST Webbook
log10ws	-1.50		Aqueous Solubility Prediction Method

logp	1.567		Crippen Method
mvol	66.330	ml/mol	McGowan Method
pc	5140.00	kPa	KDB
tb	343.70	K	NIST Webbook
tb	343.50 ± 0.50	K	NIST Webbook
tb	344.00	K	NIST Webbook
tb	343.30	K	NIST Webbook
tb	344.00 ± 0.50	K	NIST Webbook
tb	343.15 ± 0.30	K	NIST Webbook
tb	344.00 ± 4.00	K	NIST Webbook
tb	343.20	K	KDB
tc	544.40	K	NIST Webbook
tc	540.20	K	KDB
tf	154.05	K	Aqueous Solubility Prediction Method
tf	154.00	K	KDB
tf	153.75 ± 0.30	K	NIST Webbook
tf	154.15 ± 0.60	K	NIST Webbook
vc	0.246	m ³ /kmol	KDB
zc	0.2820910		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.72	J/molxK	394.21	Joback Method
cpg	112.60	J/molxK	520.87	Joback Method
cpg	108.52	J/molxK	489.20	Joback Method
cpg	104.18	J/molxK	457.54	Joback Method
cpg	99.59	J/molxK	425.87	Joback Method
cpg	84.11	J/molxK	330.88	Joback Method
cpg	89.57	J/molxK	362.54	Joback Method
dvisc	0.0015195	Paxs	206.49	Joback Method
dvisc	0.0009953	Paxs	231.37	Joback Method
dvisc	0.0007077	Paxs	256.25	Joback Method
dvisc	0.0005346	Paxs	281.12	Joback Method
dvisc	0.0004226	Paxs	306.00	Joback Method
dvisc	0.0026050	Paxs	181.61	Joback Method
dvisc	0.0003461	Paxs	330.88	Joback Method
hvapt	30.40 ± 0.10	kJ/mol	341.00	NIST Webbook
hvapt	31.00 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	31.70 ± 0.10	kJ/mol	318.00	NIST Webbook

hvapt	32.20	kJ/mol	317.50	NIST Webbook
hvapt	30.24	kJ/mol	343.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48222e+01
Coeff. B	-3.24359e+03
Coeff. C	-2.57210e+01
Temperature range (K), min.	248.88
Temperature range (K), max.	366.77

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	5.18997e+01
Coeff. B	-5.28376e+03
Coeff. C	-5.55985e+00
Coeff. D	4.84143e-06
Temperature range (K), min.	290.15
Temperature range (K), max.	540.20

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1737.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106956&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1737
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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