Propane, 2-bromo-2-methyl-

Other names:	1,1-Dimethylethyl bromide
	2-Bromo-2-methylpropane
	2-Bromoisobutane
	2-Methyl-2-bromopropane
	Bromotrimethylmethane
	Butylbromide, tert-
	NSC 8418
	Tertiarybutyl bromide
	Trimethylbromomethane
	t-Butyl bromide
	tert-Butyl bromide
	tert-C4H9Br
Inchi:	InChI=1S/C4H9Br/c1-4(2,3)5/h1-3H3
InchiKey:	RKSOPLXZQNSWAS-UHFFFAOYSA-N
Formula:	C4H9Br
SMILES:	CC(C)(C)Br
Mol. weight [g/mol]:	137.02
CAS:	507-19-7

Physical Properties

Property code	Value	Unit	Source
gf	-0.04	kJ/mol	Joback Method
hf	-132.40 ± 1.50	kJ/mol	NIST Webbook
hfl	-164.00	kJ/mol	NIST Webbook
hfl	-133.40	kJ/mol	NIST Webbook
hfus	3.99	kJ/mol	Joback Method
hvap	31.80 ± 0.10	kJ/mol	NIST Webbook
hvap	31.00	kJ/mol	NIST Webbook
hvap	31.93	kJ/mol	NIST Webbook
hvap	31.00 ± 0.84	kJ/mol	NIST Webbook
hvap	31.81 ± 0.12	kJ/mol	NIST Webbook
ie	9.95 ± 0.01	eV	NIST Webbook
ie	9.89 ± 0.03	eV	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	9.92 ± 0.03	eV	NIST Webbook

log10ws	-2.04		Crippen Method
logp	2.180		Crippen Method
mcvol	84.720	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	603.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	632.00		NIST Webbook
tb	348.00	K	NIST Webbook
tb	346.40	K	NIST Webbook
tb	346.00 ± 2.00	K	NIST Webbook
tb	346.10 ± 0.30	K	NIST Webbook
tb	346.40	K	NIST Webbook
tc	552.68	K	Joback Method
tf	256.20 ± 0.20	K	NIST Webbook
tf	256.95 ± 0.40	K	NIST Webbook
tf	146.00 ± 3.00	K	NIST Webbook
tf	246.05 ± 0.30	K	NIST Webbook
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.78	J/mol×K	453.27	Joback Method
cpg	137.79	J/mol×K	386.99	Joback Method
cpg	128.42	J/mol×K	353.85	Joback Method
cpg	162.45	J/mol×K	486.41	Joback Method
cpg	169.62	J/mol×K	519.55	Joback Method
cpg	176.32	J/mol×K	552.68	Joback Method
cpg	146.57	J/mol×K	420.13	Joback Method
cpl	165.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0032219	Pa×s	223.19	Joback Method
dvisc	0.0018233	Pa×s	249.32	Joback Method
dvisc	0.0011495	Pa×s	275.46	Joback Method
dvisc	0.0007850	Pa×s	301.59	Joback Method
dvisc	0.0005697	Pa×s	327.72	Joback Method
dvisc	0.0066215	Pa×s	197.06	Joback Method

dvisc	0.0004335	Pa×s	353.85	Joback Method
hfust	1.97	kJ/mol	256.10	NIST Webbook
hfust	1.05	kJ/mol	231.50	NIST Webbook
hfust	5.65	kJ/mol	208.60	NIST Webbook
hfust	1.97	kJ/mol	256.10	NIST Webbook
hvapt	29.23	kJ/mol	346.40	NIST Webbook
hvapt	31.40	kJ/mol	297.00	NIST Webbook
hvapt	31.20	kJ/mol	309.50	NIST Webbook
hvapt	31.50	kJ/mol	310.50	NIST Webbook
sfust	7.68	J/mol×K	256.10	NIST Webbook
sfust	4.52	J/mol×K	231.50	NIST Webbook
sfust	27.08	J/mol×K	208.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48023e+01
Coeff. B	-3.38330e+03
Coeff. C	-1.41810e+01
Temperature range (K), min.	247.28
Temperature range (K), max.	370.66

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C507197&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/ci990307l

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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume