Propane, 1-bromo-2-methyl-

Other names:	1-Bromo-2-methylpropane
	Isobutyl bromide
	UN 2342
	i-Butyl bromide
	iso-C4H9Br
Inchi:	InChI=1S/C4H9Br/c1-4(2)3-5/h4H,3H2,1-2H3
InchiKey:	HLVFKOKELQSXIQ-UHFFFAOYSA-N
Formula:	C4H9Br
SMILES:	CC(C)CBr
Mol. weight [g/mol]:	137.02
CAS:	78-77-3

Physical Properties

Property code	Value	Unit	Source
gf	-5.32	kJ/mol	Joback Method
hf	-104.84	kJ/mol	Joback Method
hfl	-160.00	kJ/mol	NIST Webbook
hfus	7.88	kJ/mol	Joback Method
hvap	34.90 ± 0.10	kJ/mol	NIST Webbook
hvap	34.90	kJ/mol	NIST Webbook
hvap	34.90 ± 0.02	kJ/mol	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
ie	10.09 ± 0.02	eV	NIST Webbook
ie	10.09 ± 0.02	eV	NIST Webbook
log10ws	-2.43		Aqueous Solubility Prediction Method
log10ws	-2.43		Estimated Solubility Method
logp	2.037		Crippen Method
mcvol	84.720	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	677.00		NIST Webbook

rinpol	686.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	671.00		NIST Webbook
tb	364.90	K	NIST Webbook
tb	364.55 ± 0.25	K	NIST Webbook
tb	364.00 ± 1.00	K	NIST Webbook
tb	364.10 ± 0.50	K	NIST Webbook
tb	364.55 ± 0.50	K	NIST Webbook
tb	364.10 ± 0.50	K	NIST Webbook
tb	364.25 ± 0.30	K	NIST Webbook
tb	364.30	K	NIST Webbook
tb	364.60 ± 0.70	K	NIST Webbook
tb	364.20 ± 0.50	K	NIST Webbook
tc	567.20	K	NIST Webbook
tf	155.10 ± 0.20	K	NIST Webbook
tf	155.15 ± 0.50	K	NIST Webbook
tf	155.80 ± 0.40	K	NIST Webbook
tf	155.00 ± 2.00	K	NIST Webbook
tf	155.75 ± 1.00	K	NIST Webbook
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	127.42	J/mol×K	356.64	Joback Method
cpg	170.96	J/mol×K	546.81	Joback Method
cpg	164.55	J/mol×K	515.12	Joback Method
cpg	157.82	J/mol×K	483.42	Joback Method
cpg	150.76	J/mol×K	451.73	Joback Method
cpg	143.34	J/mol×K	420.03	Joback Method
cpg	135.57	J/mol×K	388.34	Joback Method
cpl	154.40	J/mol×K	298.00	NIST Webbook
cpl	163.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0026265	Pa×s	209.14	Joback Method
dvisc	0.0014461	Pa×s	238.64	Joback Method
dvisc	0.0009079	Pa×s	268.14	Joback Method
dvisc	0.0006251	Pa×s	297.64	Joback Method
dvisc	0.0004604	Pa×s	327.14	Joback Method
dvisc	0.0058035	Pa×s	179.64	Joback Method
dvisc	0.0003566	Pa×s	356.64	Joback Method
hvapt	31.40 ± 0.10	kJ/mol	366.00	NIST Webbook
hvapt	32.00 ± 0.10	kJ/mol	353.00	NIST Webbook
hvapt	32.60 ± 0.10	kJ/mol	341.00	NIST Webbook
hvapt	33.10 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	34.00	kJ/mol	342.50	NIST Webbook
hvapt	34.10	kJ/mol	334.00	NIST Webbook
hvapt	31.33	kJ/mol	364.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48022e+01
Coeff. B	-3.37619e+03
Coeff. C	-3.27760e+01
Temperature range (K), min.	265.38
Temperature range (K), max.	388.51

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78773&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume