Butane, 1-bromo-3-methyl-

Other names:	1-Bromo-3-methylbutane
	3-Methylbutyl bromide
	4-Bromo-2-methylbutane
	BrCH2CH2CH(CH3)2
	ISO-AMYL BROMIDE
	Isoamyl bromide
	Isopentyl bromide
	UN 2341
Inchi:	InChI=1S/C5H11Br/c1-5(2)3-4-6/h5H,3-4H2,1-2H3
InchiKey:	YXZFFTJAHVMMLF-UHFFFAOYSA-N
Formula:	C5H11Br
SMILES:	CC(C)CCBr
Mol. weight [g/mol]:	151.04
CAS:	107-82-4

Physical Properties

Property code	Value	Unit	Source
gf	3.10	kJ/mol	Joback Method
hf	-125.48	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-2.89		Aqueous Solubility Prediction Method
logp	2.427		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	794.00		NIST Webbook
ripol	1002.00		NIST Webbook
ripol	991.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	1002.00		NIST Webbook
tb	393.40 ± 5.00	K	NIST Webbook

tb	393.80 ± 0.40	K	NIST Webbook
tb	393.45 ± 0.30	K	NIST Webbook
tb	394.60 ± 0.50	K	NIST Webbook
tb	393.75 ± 0.50	K	NIST Webbook
tb	393.50 ± 0.50	K	NIST Webbook
tb	393.50 ± 0.50	K	NIST Webbook
tb	393.80 ± 0.40	K	NIST Webbook
tb	393.50 ± 0.50	K	NIST Webbook
tb	393.75 ± 0.40	K	NIST Webbook
tb	392.00 ± 4.00	K	NIST Webbook
tb	393.80 ± 0.50	K	NIST Webbook
tb	393.60	K	NIST Webbook
tb	393.50 ± 0.50	K	NIST Webbook
tc	568.83	K	Joback Method
tf	190.91	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.34	J/mol×K	537.28	Joback Method
cpg	197.35	J/mol×K	505.73	Joback Method
cpg	212.94	J/mol×K	568.83	Joback Method
cpg	161.30	J/mol×K	379.52	Joback Method
cpg	170.96	J/mol×K	411.07	Joback Method
cpg	180.18	J/mol×K	442.62	Joback Method
cpg	188.97	J/mol×K	474.18	Joback Method
cpl	187.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0003481	Pa×s	379.52	Joback Method
dvisc	0.0006202	Pa×s	316.65	Joback Method
dvisc	0.0004527	Pa×s	348.08	Joback Method
dvisc	0.0061616	Pa×s	190.91	Joback Method
dvisc	0.0027207	Pa×s	222.34	Joback Method
dvisc	0.0014710	Pa×s	253.78	Joback Method
dvisc	0.0009108	Pa×s	285.21	Joback Method
hvapt	36.60	kJ/mol	394.60	NIST Webbook
hvapt	41.00	kJ/mol	323.00	NIST Webbook
hvapt	37.90	kJ/mol	371.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47040e+01
Coeff. B	-3.55550e+03
Coeff. C	-4.14710e+01
Temperature range (K), min.	288.10
Temperature range (K), max.	420.02

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.26440e+01
Coeff. B	-7.33684e+03
Coeff. C	-1.01195e+01
Coeff. D	6.99212e-06
Temperature range (K), min.	306.15
Temperature range (K), max.	436.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107824&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1621

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1621.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

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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume