Butane, 2-bromo-

Other names:	(+/-)-2-Bromobutane
	2-BROMOBUTANE
	2-Butyl bromide
	METHYLETHYLBROMOMETHANE
	SEC-BUTYL BROMIDE
	UN 2339
	sec-C4H9Br
Inchi:	InChI=1S/C4H9Br/c1-3-4(2)5/h4H,3H2,1-2H3
InchiKey:	UPSXAPQYNGXVBF-UHFFFAOYSA-N
Formula:	C4H9Br
SMILES:	CCC(C)Br
Mol. weight [g/mol]:	137.02
CAS:	78-76-2

Physical Properties

Property code	Value	Unit	Source
af	0.3080		KDB
chl	-2705.00 ± 1.00	kJ/mol	NIST Webbook
gf	-5.32	kJ/mol	Joback Method
hf	-120.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-156.00	kJ/mol	NIST Webbook
hfl	-155.30 ± 1.30	kJ/mol	NIST Webbook
hfus	7.88	kJ/mol	Joback Method
hvap	34.47 ± 0.06	kJ/mol	NIST Webbook
hvap	34.50 ± 0.10	kJ/mol	NIST Webbook
hvap	34.51	kJ/mol	NIST Webbook
hvap	34.80 ± 0.10	kJ/mol	NIST Webbook
hvap	34.40 ± 0.08	kJ/mol	NIST Webbook
ie	10.04	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.03	eV	NIST Webbook
ie	9.98 ± 0.01	eV	NIST Webbook
ie	10.01 ± 0.02	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.180		Crippen Method
mcvol	84.720	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB

nfpah	%!d(float64=2)		KDB
pc	4300.00	kPa	KDB
rinpol	674.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	692.00		NIST Webbook
ripol	890.00		NIST Webbook
ripol	905.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	913.00		NIST Webbook
tb	364.20	K	NIST Webbook
tb	364.00	K	NIST Webbook
tb	363.00 ± 2.00	K	NIST Webbook
tb	364.40	K	KDB
tb	364.50	K	NIST Webbook
tb	364.40 ± 0.50	K	NIST Webbook
tb	364.45 ± 0.20	K	NIST Webbook
tb	363.00 ± 2.00	K	NIST Webbook
tb	364.00	K	NIST Webbook
tc	558.70	K	KDB
tf	161.00	K	KDB
tf	160.50 ± 0.02	K	NIST Webbook
vc	0.316	m3/kmol	KDB
zc	0.2920470		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.57	J/mol×K	388.34	Joback Method
cpg	143.34	J/mol×K	420.03	Joback Method
cpg	150.76	J/mol×K	451.73	Joback Method
cpg	170.96	J/mol×K	546.81	Joback Method
cpg	157.82	J/mol×K	483.42	Joback Method
cpg	164.55	J/mol×K	515.12	Joback Method
cpg	127.42	J/mol×K	356.64	Joback Method

dvisc	0.0004604	Pa×s	327.14	Joback Method
dvisc	0.0006251	Pa×s	297.64	Joback Method
dvisc	0.0009079	Pa×s	268.14	Joback Method
dvisc	0.0014461	Pa×s	238.64	Joback Method
dvisc	0.0026265	Pa×s	209.14	Joback Method
dvisc	0.0003566	Pa×s	356.64	Joback Method
dvisc	0.0058035	Pa×s	179.64	Joback Method
hfust	6.88	kJ/mol	160.30	NIST Webbook
hfust	6.88	kJ/mol	160.30	NIST Webbook
hvapt	33.90	kJ/mol	342.00	NIST Webbook
hvapt	30.77	kJ/mol	364.50	NIST Webbook
hvapt	32.76	kJ/mol	364.40	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46914e+01
Coeff. B	-3.31459e+03
Coeff. C	-3.49450e+01
Temperature range (K), min.	265.06
Temperature range (K), max.	388.32

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.51791e+01
Coeff. B	-6.62032e+03
Coeff. C	-9.03951e+00
Coeff. D	6.95378e-06
Temperature range (K), min.	161.25
Temperature range (K), max.	567.00

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78762&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=1607
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1607

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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
zc:	Critical Compressibility

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.