Propane, 2-bromo-

Other names:	2-Bromopropane
	ISOPROPYL BROMIDE
	SEC-PROPYL BROMIDE
	UN 2344
	iso-C3H7Br
Inchi:	InChI=1S/C3H7Br/c1-3(2)4/h3H,1-2H3
InchiKey:	NAMYKGVDVNBCFQ-UHFFFAOYSA-N
Formula:	C3H7Br
SMILES:	CC(C)Br
Mol. weight [g/mol]:	122.99
CAS:	75-26-3

Physical Properties

Property code	Value	Unit	Source
chl	-2051.90 ± 1.80	kJ/mol	NIST Webbook
gf	-13.74	kJ/mol	Joback Method
hf	-95.60 ± 1.00	kJ/mol	NIST Webbook
hf	-98.50 ± 1.90	kJ/mol	NIST Webbook
hf	-98.50 ± 1.90	kJ/mol	NIST Webbook
hfl	-129.10 ± 1.80	kJ/mol	NIST Webbook
hfl	-129.00	kJ/mol	NIST Webbook
hfus	5.29	kJ/mol	Joback Method
hvap	30.33	kJ/mol	NIST Webbook
hvap	30.20 ± 0.10	kJ/mol	NIST Webbook
hvap	30.20 ± 0.08	kJ/mol	NIST Webbook
hvap	30.60	kJ/mol	NIST Webbook
ie	10.13	eV	NIST Webbook
ie	10.12 ± 0.01	eV	NIST Webbook
ie	10.40 ± 0.10	eV	NIST Webbook
ie	10.07	eV	NIST Webbook
ie	10.10 ± 0.02	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.08 ± 0.01	eV	NIST Webbook
log10ws	-1.59		Estimated Solubility Method
log10ws	-1.59		Aqueous Solubility Prediction Method

logp	1.790		Crippen Method
mcvol	70.630	ml/mol	McGowan Method
pc	4897.06	kPa	Joback Method
rinpol	565.00		NIST Webbook
rinpol	571.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	571.00		NIST Webbook
tb	332.50 ± 0.50	K	NIST Webbook
tb	334.65 ± 2.00	K	NIST Webbook
tb	334.70 ± 0.80	K	NIST Webbook
tb	332.60 ± 0.15	K	NIST Webbook
tb	333.00 ± 0.50	K	NIST Webbook
tb	332.65 ± 0.60	K	NIST Webbook
tb	332.50	K	KDB
tb	332.60	K	NIST Webbook
tb	332.32 ± 0.20	K	NIST Webbook
tb	332.60 ± 0.60	K	NIST Webbook
tb	332.70 ± 0.30	K	NIST Webbook
tb	332.00 ± 2.00	K	NIST Webbook
tb	332.61 ± 0.20	K	NIST Webbook
tb	332.60	K	NIST Webbook
tb	332.60 ± 0.50	K	NIST Webbook
tb	332.80 ± 0.50	K	NIST Webbook
tc	532.00	K	NIST Webbook
tf	184.05 ± 0.50	K	NIST Webbook
tf	184.55 ± 0.50	K	NIST Webbook
tf	184.15	K	KDB
tf	184.20 ± 0.30	K	NIST Webbook
vc	0.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	130.79	J/mol×K	524.35	Joback Method
cpg	102.61	J/mol×K	365.53	Joback Method
cpg	108.81	J/mol×K	397.29	Joback Method
cpg	114.71	J/mol×K	429.06	Joback Method
cpg	120.34	J/mol×K	460.82	Joback Method
cpg	125.69	J/mol×K	492.59	Joback Method
cpg	96.11	J/mol×K	333.76	Joback Method
cpl	135.60	J/mol×K	298.15	NIST Webbook
cpl	126.80	J/mol×K	209.60	NIST Webbook
cpl	132.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0004194	Pa×s	318.15	Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K
dvisc	0.0004389	Pa×s	313.15	Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K
dvisc	0.0004708	Pa×s	308.15	Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K
dvisc	0.0004835	Pa×s	303.15	Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K

dvisc	0.0004981	Pa×s	298.15	Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K
hfust	6.53	kJ/mol	184.10	NIST Webbook
hfust	6.55	kJ/mol	184.10	NIST Webbook
hfust	6.53	kJ/mol	184.10	NIST Webbook
hvapt	33.40	kJ/mol	272.00	NIST Webbook
hvapt	28.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	29.20 ± 0.10	kJ/mol	318.00	NIST Webbook
hvapt	29.80 ± 0.10	kJ/mol	305.00	NIST Webbook
hvapt	30.10	kJ/mol	315.50	NIST Webbook
hvapt	32.10	kJ/mol	282.00	NIST Webbook
hvapt	28.33	kJ/mol	332.60	NIST Webbook
hvapt	30.90	kJ/mol	288.00	NIST Webbook
hvapt	28.40	kJ/mol	331.60	NIST Webbook
hvapt	28.00 ± 0.10	kJ/mol	338.00	NIST Webbook
sfust	35.50	J/mol×K	184.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46798e+01
Coeff. B	-3.07460e+03
Coeff. C	-2.74180e+01
Temperature range (K), min.	241.05
Temperature range (K), max.	355.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.00355e+01
Coeff. B	-5.73559e+03
Coeff. C	-8.46248e+00
Coeff. D	8.75295e-06

Temperature range (K), min.	184.15
Temperature range (K), max.	532.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurement and Correlation of the Densities and Viscosities of 2-Bromopropane + Ethanol Binary Mixtures at Temperatures from (298.15 to 318.15) K:	https://www.doi.org/10.1021/je100159m
Abraham model linear free energy relationships for describing the partitioning and solubility behavior of nonelectrolyte organic solutes dissolved in pyridine at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2016.10.009
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75263&Units=SI
Measurement and Correlation for Solubility of 2-Bromopropane and Thiourea in Water:	https://www.doi.org/10.1021/je800796h
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1593
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1593.mol

Legend

chl:	Standard liquid enthalpy of combustion
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