Ethyl bromide

Other names:	1-Bromoethane
	BROMIC ETHER
	Bromoethane
	Bromure d'ethyle
	C2H5Br
	Ethane, bromo-
	Etylu bromek
	Halon 2001
	Hydrobromic ether
	Monobromoethane
	NCI-C55481
	NSC 8824
	UN 1891
Inchi:	InChI=1S/C2H5Br/c1-2-3/h2H2,1H3
InchiKey:	RDHPKYGYEGBMSE-UHFFFAOYSA-N
Formula:	C2H5Br
SMILES:	CCBr
Mol. weight [g/mol]:	108.97
CAS:	74-96-4

Physical Properties

Property code	Value	Unit	Source
af	0.2290		KDB
affp	684.30 ± 1.60	kJ/mol	NIST Webbook
affp	696.20	kJ/mol	NIST Webbook
basg	669.70	kJ/mol	NIST Webbook
basg	660.50 ± 1.60	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
ep	29.20	J/mol×K	NIST Webbook
gf	-26.33	kJ/mol	KDB
hf	-65.30 ± 6.30	kJ/mol	NIST Webbook
hf	-64.06	kJ/mol	KDB
hf	-61.90 ± 1.00	kJ/mol	NIST Webbook
hf	-64.60 ± 2.10	kJ/mol	NIST Webbook
hf	-63.60	kJ/mol	NIST Webbook
hfl	-95.50 ± 2.10	kJ/mol	NIST Webbook
hfus	6.22	kJ/mol	Joback Method

hvap	28.00 ± 1.00	kJ/mol	NIST Webbook
hvap	28.26	kJ/mol	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.29 ± 0.02	eV	NIST Webbook
ie	10.29 ± 0.01	eV	NIST Webbook
ie	10.30 ± 0.01	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.29 ± 0.01	eV	NIST Webbook
ie	10.28	eV	NIST Webbook
ie	10.29	eV	NIST Webbook
ie	10.28	eV	NIST Webbook
ie	10.24 ± 0.03	eV	NIST Webbook
ie	10.31	eV	NIST Webbook
log10ws	-1.09		Estimated Solubility Method
log10ws	-1.09		Aqueous Solubility Prediction Method
logp	1.401		Crippen Method
mcvol	56.540	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	6230.00	kPa	KDB
pc	6231.49 ± 81.06	kPa	NIST Webbook
rhoc	506.69 ± 3.27	kg/m3	NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	529.00		NIST Webbook
rinpol	509.60		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	529.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	509.60		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	524.00		NIST Webbook
ripol	777.51		NIST Webbook
ripol	784.00		NIST Webbook

ripol	792.57		NIST Webbook
ripol	792.57		NIST Webbook
ripol	783.00		NIST Webbook
ripol	776.00		NIST Webbook
ripol	795.84		NIST Webbook
tb	311.60	K	KDB
tc	503.95 ± 0.40	K	NIST Webbook
tc	503.80	K	NIST Webbook
tc	503.90	K	KDB
tf	154.23	K	Aqueous Solubility Prediction Method
tf	154.50	K	KDB
vc	0.215	m3/kmol	KDB
zc	0.3197020		KDB
zra	0.29		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	67.74	J/mol×K	311.32	Joback Method
cpg	72.22	J/mol×K	342.25	Joback Method
cpg	76.49	J/mol×K	373.18	Joback Method
cpg	80.56	J/mol×K	404.11	Joback Method
cpg	84.44	J/mol×K	435.03	Joback Method
cpg	88.14	J/mol×K	465.96	Joback Method
cpg	91.66	J/mol×K	496.89	Joback Method
cpl	104.85	J/mol×K	276.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	104.37	J/mol×K	271.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	104.60	J/mol×K	274.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	104.07	J/mol×K	269.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	105.14	J/mol×K	279.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	105.42	J/mol×K	281.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	105.63	J/mol×K	284.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	105.91	J/mol×K	286.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	106.14	J/mol×K	289.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	106.42	J/mol×K	291.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	106.75	J/mol×K	294.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	107.09	J/mol×K	296.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	107.42	J/mol×K	299.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	100.80	J/mol×K	298.00	NIST Webbook	
cpl	105.80	J/mol×K	298.15	NIST Webbook	
dvisc	0.0027010	Pa×s	172.10	Joback Method	
dvisc	0.0015726	Pa×s	195.30	Joback Method	
dvisc	0.0010270	Pa×s	218.51	Joback Method	
dvisc	0.0007279	Pa×s	241.71	Joback Method	

dvisc	0.0005480	Pa×s	264.91	Joback Method
dvisc	0.0004318	Pa×s	288.12	Joback Method
dvisc	0.0003526	Pa×s	311.32	Joback Method
hvapt	26.90	kJ/mol	419.00	NIST Webbook
hvapt	27.90	kJ/mol	324.50	NIST Webbook
hvapt	26.48	kJ/mol	311.70	KDB
hvapt	26.60	kJ/mol	390.00	NIST Webbook
hvapt	31.00	kJ/mol	477.50	NIST Webbook
hvapt	30.60	kJ/mol	279.00	NIST Webbook
hvapt	27.60 ± 0.10	kJ/mol	305.00	NIST Webbook
hvapt	27.00 ± 0.10	kJ/mol	312.00	NIST Webbook
hvapt	26.20 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	27.04	kJ/mol	311.60	NIST Webbook
rhol	1451.01	kg/m3	298.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48270e+01
Coeff. B	-2.90222e+03
Coeff. C	-2.72110e+01
Temperature range (K), min.	226.82
Temperature range (K), max.	503.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.12149e+01
Coeff. B	-5.79769e+03
Coeff. C	-1.03099e+01
Coeff. D	1.24422e-05
Temperature range (K), min.	154.55
Temperature range (K), max.	503.80

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1577.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74964&Units=SI
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1577
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis:	https://www.doi.org/10.1021/je049652j
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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ep:	Protonation entropy at 298K
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter