Propane, 1,2-dibromo-

Other names:	.+/-.-1,2-Dibromopropane
	1,2-Dibromopropane
	CH2BrCHBrCH3
	Propylene dibromide
Inchi:	InChI=1S/C3H6Br2/c1-3(5)2-4/h3H,2H2,1H3
InchiKey:	XFNJYAKDBJUJAJ-UHFFFAOYSA-N
Formula:	C3H6Br2
SMILES:	CC(Br)CBr
Mol. weight [g/mol]:	201.89
CAS:	78-75-1

Physical Properties

Property code	Value	Unit	Source
af	0.3840		KDB
gf	0.58	kJ/mol	Joback Method
hf	-57.87	kJ/mol	Joback Method
hfus	10.57	kJ/mol	Joback Method
hvap	42.20	kJ/mol	NIST Webbook
hvap	42.30 ± 0.70	kJ/mol	NIST Webbook
hvap	41.69	kJ/mol	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.38	eV	NIST Webbook
log10ws	-2.15		Aqueous Solubility Prediction Method
logp	2.165		Crippen Method
mcvol	88.130	ml/mol	McGowan Method
pc	5410.00	kPa	KDB
rinpol	846.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	823.00		NIST Webbook
tb	413.20	K	KDB
tb	415.20 ± 1.00	K	NIST Webbook

tb	414.00 ± 3.00	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	413.00 ± 2.00	K	NIST Webbook
tb	414.00 ± 4.00	K	NIST Webbook
tb	415.00 ± 2.00	K	NIST Webbook
tb	414.00 ± 3.00	K	NIST Webbook
tb	413.05 ± 0.20	K	NIST Webbook
tb	415.00 ± 6.00	K	NIST Webbook
tb	416.65 ± 4.00	K	NIST Webbook
tb	416.15 ± 5.00	K	NIST Webbook
tb	416.40 ± 2.00	K	NIST Webbook
tb	413.00 ± 4.00	K	NIST Webbook
tb	415.00	K	NIST Webbook
tb	413.20	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	413.00 ± 2.00	K	NIST Webbook
tc	634.10	K	KDB
tf	217.90 ± 0.20	K	NIST Webbook
tf	218.00	K	KDB
tf	217.99	K	Aqueous Solubility Prediction Method
tf	217.70 ± 0.02	K	NIST Webbook
vc	0.322	m3/kmol	KDB
zc	0.3299010		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.65	J/mol×K	506.85	Joback Method
cpg	136.01	J/mol×K	471.21	Joback Method
cpg	156.45	J/mol×K	613.78	Joback Method
cpg	151.84	J/mol×K	578.14	Joback Method
cpg	146.92	J/mol×K	542.50	Joback Method
cpg	123.53	J/mol×K	399.92	Joback Method
cpg	129.98	J/mol×K	435.56	Joback Method
cpl	172.80	J/mol×K	298.00	NIST Webbook
dvisc	0.0024124	Pa×s	256.80	Joback Method
dvisc	0.0015096	Pa×s	285.42	Joback Method
dvisc	0.0010289	Pa×s	314.05	Joback Method
dvisc	0.0007477	Pa×s	342.67	Joback Method
dvisc	0.0005708	Pa×s	371.30	Joback Method

dvisc	0.0043363	Pa×s	228.17	Joback Method
dvisc	0.0004529	Pa×s	399.92	Joback Method
hvapt	42.80	kJ/mol	340.50	NIST Webbook
hvapt	44.60	kJ/mol	392.50	NIST Webbook
hvapt	41.40	kJ/mol	357.50	NIST Webbook
hvapt	35.61	kJ/mol	415.00	NIST Webbook
hvapt	41.01	kJ/mol	413.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48599e+01
Coeff. B	-3.61999e+03
Coeff. C	-6.05390e+01
Temperature range (K), min.	308.96
Temperature range (K), max.	439.66

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.84620e+01
Coeff. B	-8.51840e+03
Coeff. C	-1.23841e+01
Coeff. D	7.75533e-06
Temperature range (K), min.	266.15
Temperature range (K), max.	525.15

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1585

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78751&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=1585

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
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
zc:	Critical Compressibility