Vinyl bromide

Other names:	Bromoethene
	Bromoethylene
	Bromure de vinyle
	C2H3Br
	Ethene, bromo-
	Ethylene, bromo-
	NCI-C50373
	Saytex VBR
	UN 1085
	Vinylbromid
Inchi:	InChI=1S/C2H3Br/c1-2-3/h2H,1H2
InchiKey:	INLLPKCGLOXCIV-UHFFFAOYSA-N
Formula:	C2H3Br
SMILES:	C=CBr
Mol. weight [g/mol]:	106.95
CAS:	593-60-2

Physical Properties

Property code	Value	Unit	Source
gf	68.12	kJ/mol	Joback Method
hf	79.20 ± 1.90	kJ/mol	NIST Webbook
hfus	4.94	kJ/mol	Joback Method
hvap	25.81	kJ/mol	Joback Method
ie	9.82 ± 0.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.80 ± 0.01	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.80 ± 0.02	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.87	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.90 ± 0.01	eV	NIST Webbook
ie	9.82 ± 0.03	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.525		Crippen Method
mcvol	52.240	ml/mol	McGowan Method

pc	5926.27	kPa	Joback Method
rinpol	450.00		NIST Webbook
rinpol	450.00		NIST Webbook
tb	289.00	K	NIST Webbook
tb	289.00	K	NIST Webbook
tc	497.75	K	Joback Method
tf	133.61 ± 0.02	K	NIST Webbook
vc	0.191	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	75.28	J/mol×K	497.75	Joback Method
cpg	69.79	J/mol×K	434.50	Joback Method
cpg	72.62	J/mol×K	466.13	Joback Method
cpg	56.43	J/mol×K	308.00	Joback Method
cpg	60.10	J/mol×K	339.63	Joback Method
cpg	63.54	J/mol×K	371.25	Joback Method
cpg	66.77	J/mol×K	402.88	Joback Method
cpl	107.90	J/mol×K	288.00	NIST Webbook
cpl	107.50	J/mol×K	288.00	NIST Webbook
dvisc	0.0003301	Pa×s	308.00	Joback Method
dvisc	0.0004965	Pa×s	262.11	Joback Method
dvisc	0.0003982	Pa×s	285.06	Joback Method
dvisc	0.0021737	Pa×s	170.34	Joback Method
dvisc	0.0013176	Pa×s	193.28	Joback Method
dvisc	0.0008882	Pa×s	216.23	Joback Method
dvisc	0.0006458	Pa×s	239.17	Joback Method
hvapt	26.90	kJ/mol	246.00	NIST Webbook
hvapt	24.80	kJ/mol	237.50	NIST Webbook
hvapt	27.30	kJ/mol	271.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	289.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.54408e+01
Coeff. B	-3.96182e+03
Coeff. C	-4.91163e+00
Coeff. D	8.60843e-06
Temperature range (K), min.	135.35
Temperature range (K), max.	473.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1730
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/files/research/kdb/mol/mol1730.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C593602&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume