1-Propene, 2,3-dibromo-

Other names:	1,2-Dibromo-2-propene
	2,3-Dibromo-1-propene
	2,3-Dibromopropene
	2,3-Dibromopropylene
	2-Bromoallyl bromide
	Propene, 2,3-dibromo-
Inchi:	InChI=1S/C3H4Br2/c1-3(5)2-4/h1-2H2
InchiKey:	YMFWYDYJHRGGPF-UHFFFAOYSA-N
Formula:	C3H4Br2
SMILES:	C=C(Br)CBr
Mol. weight [g/mol]:	199.87
CAS:	513-31-5

Physical Properties

Property code	Value	Unit	Source
gf	82.31	kJ/mol	Joback Method
hf	63.05	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	34.55	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.290		Crippen Method
mcvol	83.830	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
tb	414.20	K	NIST Webbook
tc	614.99	K	Joback Method
tf	227.45	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.30	J/mol×K	578.64	Joback Method

cpg	109.41	J/mol×K	396.92	Joback Method
cpg	114.78	J/mol×K	433.26	Joback Method
cpg	119.72	J/mol×K	469.61	Joback Method
cpg	124.27	J/mol×K	505.95	Joback Method
cpg	128.45	J/mol×K	542.30	Joback Method
cpg	135.86	J/mol×K	614.99	Joback Method
hvapt	43.10	kJ/mol	341.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	316.20	K	2.30	NIST Webbook
tbrp	316.00 ± 1.00	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49338e+01
Coeff. B	-3.87999e+03
Coeff. C	-3.80660e+01
Temperature range (K), min.	302.98
Temperature range (K), max.	441.30

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C513315&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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