1-Bromo-2-methylpropene

Other names:	1-Bromo-2-methyl-1-propene
	1-Propene, 1-bromo-2-methyl-
	2-Methyl-1-propenyl bromide
	Isocrotyl bromide
	Propene, 1-bromo-2-methyl-
	«beta»,«beta»-Dimethylvinylbromide
	Â«betaÂ»,Â«betaÂ»-Dimethylvinylbromide
Inchi:	InChI=1S/C4H7Br/c1-4(2)3-5/h3H,1-2H3
InchiKey:	DEFNUDNHTUZJAL-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	CC(C)=CBr
Mol. weight [g/mol]:	135.00
CAS:	3017-69-4

Physical Properties

Property code	Value	Unit	Source
gf	68.79	kJ/mol	Joback Method
hf	7.87	kJ/mol	Joback Method
hfus	10.29	kJ/mol	Joback Method
hvap	30.97	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.305		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	360.00 ± 4.00	K	NIST Webbook
tc	561.25	K	Joback Method
tf	175.60	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.99	J/mol×K	361.12	Joback Method
cpg	120.59	J/mol×K	394.48	Joback Method

cpg	127.72	J/mol×K	427.83	Joback Method
cpg	134.41	J/mol×K	461.19	Joback Method
cpg	140.69	J/mol×K	494.54	Joback Method
cpg	146.58	J/mol×K	527.90	Joback Method
cpg	152.11	J/mol×K	561.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40552e+01
Coeff. B	-2.55000e+03
Coeff. C	-8.97840e+01
Temperature range (K), min.	275.00
Temperature range (K), max.	387.05

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3017694&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

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

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

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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume