Isopropenyl bromide

Other names:	1-Propene, 2-bromo-
	2-Bromo-1-propene
	2-Bromopropene
	2-Bromopropylene
	CH3CBr=CH2
	Isopropylene bromide
	NSC 87535
	Propene, 2-bromo-
	«alpha»-Methylvinyl bromide
	Â«alphaÂ»-Methylvinyl bromide
Inchi:	InChI=1S/C3H5Br/c1-3(2)4/h1H2,2H3
InchiKey:	PHMRPWPDDRGGGF-UHFFFAOYSA-N
Formula:	C3H5Br
SMILES:	C=C(C)Br
Mol. weight [g/mol]:	120.98
CAS:	557-93-7

Physical Properties

Property code	Value	Unit	Source
gf	67.99	kJ/mol	Joback Method
hf	36.72	kJ/mol	Joback Method
hfus	6.22	kJ/mol	Joback Method
hvap	28.12	kJ/mol	Joback Method
ie	9.58 ± 0.02	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	1.915		Crippen Method
mcvol	66.330	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	321.60	K	NIST Webbook
tb	321.00	K	NIST Webbook
tc	524.94	K	Joback Method
tf	167.65	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	84.18	J/mol×K	330.76	Joback Method
cpg	89.73	J/mol×K	363.12	Joback Method
cpg	94.95	J/mol×K	395.49	Joback Method
cpg	99.88	J/mol×K	427.85	Joback Method
cpg	104.52	J/mol×K	460.21	Joback Method
cpg	108.89	J/mol×K	492.57	Joback Method
cpg	113.01	J/mol×K	524.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48367e+01
Coeff. B	-3.09866e+03
Coeff. C	-1.85550e+01
Temperature range (K), min.	231.53
Temperature range (K), max.	343.87

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C557937&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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume