2-Bromo-3-chloropropene-1

Other names: 2-Bromo-3-chloro-1-propene
1-Propene, 2-bromo-3-chloro-
2-bromo-3-chloropropene
Inchi: InChI=1S/C3H4BrCl/c1-3(4)2-5/h1-2H2
InchiKey: LGQUWHWIEUSLLO-UHFFFAOYSA-N
Formula: C3H4BrCl
SMILES: C=C(Br)CCl
Mol. weight [g/mol]: 155.42
CAS: 16400-63-8

Physical Properties

Property code	Value	Unit	Source
gf	56.06	kJ/mol	Joback Method
hf	20.98	kJ/mol	Joback Method
hfus	10.42	kJ/mol	Joback Method
hvap	32.50	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.134		Crippen Method
mcvol	78.570	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	368.19	K	Joback Method
tc	572.54	K	Joback Method
tf	197.57	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.64	J/mol×K	368.19	Joback Method
cpg	108.91	J/mol×K	402.25	Joback Method
cpg	113.83	J/mol×K	436.31	Joback Method
cpg	118.42	J/mol×K	470.36	Joback Method
cpg	122.70	J/mol×K	504.42	Joback Method
cpg	126.69	J/mol×K	538.48	Joback Method

cpg	130.41	J/mol×K	572.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16400638&Units=SI

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