

Propane, 1-bromo-3-chloro-2-methyl-

Other names:	1-Bromo-3-chloro-2-methylpropane ./-.-1-Bromo-3-chloro-2-methylpropane
Inchi:	InChI=1S/C4H8BrCl/c1-4(2-5)3-6/h4H,2-3H2,1H3
InchiKey:	ZKDOQFPDSUOLGF-UHFFFAOYSA-N
Formula:	C4H8BrCl
SMILES:	CC(CCl)CBr
Mol. weight [g/mol]:	171.46
CAS:	6974-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.25	kJ/mol	Joback Method
hf	-120.58	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	34.93	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	2.256		Crippen Method
mvol	96.960	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	593.13	K	Joback Method
tf	209.56	K	Joback Method
vc	0.364	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.95	J/molxK	394.07	Joback Method
cpg	157.83	J/molxK	427.25	Joback Method
cpg	165.30	J/molxK	460.42	Joback Method
cpg	172.37	J/molxK	493.60	Joback Method
cpg	179.06	J/molxK	526.77	Joback Method
cpg	185.39	J/molxK	559.95	Joback Method
cpg	191.38	J/molxK	593.13	Joback Method

dvisc	0.0054945	Paxs	209.56	Joback Method
dvisc	0.0026714	Paxs	240.31	Joback Method
dvisc	0.0015297	Paxs	271.06	Joback Method
dvisc	0.0009813	Paxs	301.81	Joback Method
dvisc	0.0006834	Paxs	332.57	Joback Method
dvisc	0.0005060	Paxs	363.32	Joback Method
dvisc	0.0003926	Paxs	394.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6974772&Units=SI
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
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
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

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