Propane, 2-bromo-1-chloro-

Other names: 1-Chloro-2-bromopropane
2-Bromo-1-chloropropane
Inchi: InChI=1S/C3H6BrCl/c1-3(4)2-5/h3H,2H2,1H3
InchiKey: PUJJZGFFAQHYEX-UHFFFAOYSA-N
Formula: C3H6BrCl
SMILES: CC(Br)CCl
Mol. weight [g/mol]: 157.44
CAS: 3017-95-6

Physical Properties

Property code	Value	Unit	Source
gf	-25.67	kJ/mol	Joback Method
hf	-99.94	kJ/mol	Joback Method
hfus	9.48	kJ/mol	Joback Method
hvap	32.70	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	2.009		Crippen Method
mcvol	82.870	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	743.60		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	743.60		NIST Webbook
tb	389.70	K	NIST Webbook
tc	571.70	K	Joback Method
tf	198.29	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.80	J/mol×K	371.19	Joback Method
cpg	123.09	J/mol×K	404.61	Joback Method
cpg	129.03	J/mol×K	438.03	Joback Method
cpg	134.65	J/mol×K	471.44	Joback Method

cpg	139.96	J/mol×K	504.86	Joback Method
cpg	144.97	J/mol×K	538.28	Joback Method
cpg	149.70	J/mol×K	571.70	Joback Method
dvisc	0.0052743	Pa×s	198.29	Joback Method
dvisc	0.0026310	Pa×s	227.11	Joback Method
dvisc	0.0015350	Pa×s	255.92	Joback Method
dvisc	0.0009987	Pa×s	284.74	Joback Method
dvisc	0.0007032	Pa×s	313.56	Joback Method
dvisc	0.0005253	Pa×s	342.37	Joback Method
dvisc	0.0004106	Pa×s	371.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.20	K	101.00	NIST Webbook
tbrp	391.00	K	101.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3017956&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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