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

Other names: 2-bromo-6-chlorotoluene
Inchi: InChI=1S/C7H6BrCl/c1-5-6(8)3-2-4-7(5)9/h2-4H,1H3
InchiKey: DMARBQGIQKLIPM-UHFFFAOYSA-N
Formula: C7H6BrCl
SMILES: Cc1c(Cl)cccc1Br
Mol. weight [g/mol]: 205.48
CAS: 62356-27-8

Physical Properties

Property code	Value	Unit	Source
gf	103.60	kJ/mol	Joback Method
hf	36.37	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	45.60	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.411		Crippen Method
mcvol	115.470	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
tb	499.79	K	Joback Method
tc	740.87	K	Joback Method
tf	309.83	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.09	J/mol×K	499.79	Joback Method
cpg	204.33	J/mol×K	539.97	Joback Method
cpg	212.93	J/mol×K	580.15	Joback Method
cpg	220.93	J/mol×K	620.33	Joback Method
cpg	228.35	J/mol×K	660.51	Joback Method
cpg	235.24	J/mol×K	700.69	Joback Method
cpg	241.62	J/mol×K	740.87	Joback Method
dvisc	0.0015976	Pa×s	309.83	Joback Method

dvisc	0.0010646	Pa×s	341.49	Joback Method
dvisc	0.0007600	Pa×s	373.15	Joback Method
dvisc	0.0005719	Pa×s	404.81	Joback Method
dvisc	0.0004485	Pa×s	436.47	Joback Method
dvisc	0.0003635	Pa×s	468.13	Joback Method
dvisc	0.0003025	Pa×s	499.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	5.30	NIST Webbook

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=C62356278&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume