

# 4-Bromo-3-chlorotoluene

<b>Inchi:</b>	InChI=1S/C7H6BrCl/c1-5-2-3-6(8)7(9)4-5/h2-4H,1H3
<b>InchiKey:</b>	SDTULEXOSNNGAW-UHFFFAOYSA-N
<b>Formula:</b>	C7H6BrCl
<b>SMILES:</b>	Cc1ccc(Br)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	205.48
<b>CAS:</b>	6627-51-6

## 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	m <sup>3</sup> /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	Paxs	309.83	Joback Method
dvisc	0.0010646	Paxs	341.49	Joback Method

dvisc	0.0007600	Paxs	373.15	Joback Method
dvisc	0.0005719	Paxs	404.81	Joback Method
dvisc	0.0004485	Paxs	436.47	Joback Method
dvisc	0.0003635	Paxs	468.13	Joback Method
dvisc	0.0003025	Paxs	499.79	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6627516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6627516&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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