

2-Bromo-6-chlorotoluene

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

Physical Properties

Property code	Value	Unit	Source
hf	41.72	kJ/mol	Cheméo Relay (1.0)
hfus	16.63	kJ/mol	Joback Method
hvap	54.07	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-4.13		Cheméo Relay (1.0)
logp	3.411		Crippen Method
mcvol	115.470	ml/mol	McGowan Method
tb	495.64	K	Cheméo Relay (1.0)
tf	326.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.09	J/mol×K	499.79	Joback Method
cpg	241.62	J/mol×K	740.87	Joback Method
cpg	235.24	J/mol×K	700.69	Joback Method
cpg	228.35	J/mol×K	660.51	Joback Method
cpg	220.93	J/mol×K	620.33	Joback Method
cpg	212.93	J/mol×K	580.15	Joback Method
cpg	204.33	J/mol×K	539.97	Joback Method
dvisc	0.0005719	Pa×s	404.81	Joback Method
dvisc	0.0003025	Pa×s	499.79	Joback Method
dvisc	0.0003635	Pa×s	468.13	Joback Method
dvisc	0.0004485	Pa×s	436.47	Joback Method
dvisc	0.0015976	Pa×s	309.83	Joback Method

dvisc	0.0007600	Pa×s	373.15	Joback Method
dvisc	0.0010646	Pa×s	341.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62356278&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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