

Benzene, 1-bromo-4-chloro-2-methyl-

Other names:	Toluene, 2-bromo-5-chloro- 2-Bromo-5-chlorotoluene 6-Bromo-3-chlorotoluene
Inchi:	InChI=1S/C7H6BrCl/c1-5-4-6(9)2-3-7(5)8/h2-4H,1H3
InchiKey:	RTIPTGMVQIIMKL-UHFFFAOYSA-N
Formula:	C7H6BrCl
SMILES:	Cc1cc(Cl)ccc1Br
Mol. weight [g/mol]:	205.48
CAS:	14495-51-3

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 ³ /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/molxK	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	3.30	NIST Webbook
tbrp	372.00 ± 1.00	K	3.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14495513&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
mvol:	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

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