5-Bromo-2-chlorobenzoic acid

Other names: Benzoic acid, 5-bromo-2-chloro-
Inchi: InChI=1S/C7H4BrClO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)
InchiKey: FGERXQWKKIVFQG-UHFFFAOYSA-N
Formula: C7H4BrClO2
SMILES: O=C(O)c1cc(Br)ccc1Cl
Mol. weight [g/mol]: 235.46
CAS: 21739-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-162.14	kJ/mol	Joback Method
hf	-228.44	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.801		Crippen Method
mcvol	122.910	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	645.84	K	Joback Method
tc	874.04	K	Joback Method
tf	420.58	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.54	J/mol×K	645.84	Joback Method
cpg	264.88	J/mol×K	836.01	Joback Method
cpg	260.27	J/mol×K	797.98	Joback Method
cpg	255.26	J/mol×K	759.94	Joback Method
cpg	249.82	J/mol×K	721.91	Joback Method
cpg	243.93	J/mol×K	683.87	Joback Method
cpg	269.11	J/mol×K	874.04	Joback Method
dvisc	0.0000985	Pa×s	645.84	Joback Method

dvisc	0.0001353	Pa×s	608.30	Joback Method
dvisc	0.0001938	Pa×s	570.75	Joback Method
dvisc	0.0002920	Pa×s	533.21	Joback Method
dvisc	0.0004682	Pa×s	495.67	Joback Method
dvisc	0.0008109	Pa×s	458.12	Joback Method
dvisc	0.0015492	Pa×s	420.58	Joback Method

Sources

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=C21739924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume