

2-Bromo-5-chlorobenzoic acid

Other names:	6-Bromo-3-chlorobenzoic acid Benzoic acid, 2-bromo-5-chloro-
Inchi:	InChI=1S/C7H4BrClO2/c8-6-2-1-4(9)3-5(6)7(10)11/h1-3H,(H,10,11)
InchiKey:	RBCPJQQJBAQSOU-UHFFFAOYSA-N
Formula:	C7H4BrClO2
SMILES:	O=C(O)c1cc(Cl)ccc1Br
Mol. weight [g/mol]:	235.46
CAS:	21739-93-5

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0015492	Paxs	420.58	Joback Method
dvisc	0.0008109	Paxs	458.12	Joback Method
dvisc	0.0004682	Paxs	495.67	Joback Method
dvisc	0.0002920	Paxs	533.21	Joback Method
dvisc	0.0001938	Paxs	570.75	Joback Method
dvisc	0.0001353	Paxs	608.30	Joback Method
dvisc	0.0000985	Paxs	645.84	Joback Method

Sources

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=C21739935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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