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

Physical Properties

Property code	Value	Unit	Source
hf	-299.23	kJ/mol	Cheméo Relay (1.0)
hfus	22.32	kJ/mol	Joback Method
ie	9.16	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	2.801		Crippen Method
mcvol	122.910	ml/mol	McGowan Method
tb	564.91	K	Cheméo Relay (1.0)
tf	431.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.54	J/mol×K	645.84	Joback Method
cpg	269.11	J/mol×K	874.04	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
dvisc	0.0002920	Pa×s	533.21	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	0.0015492	Pa×s	420.58	Joback Method
dvisc	0.0004682	Pa×s	495.67	Joback Method

dvisc	0.0008109	Pa×s	458.12	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21739924&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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