Phenol, 2-bromo-4-chloro-

Other names: 2-Bromo-4-chlorophenol
Inchi: InChI=1S/C6H4BrClO/c7-5-3-4(8)1-2-6(5)9/h1-3,9H
InchiKey: ZIYRDJLAJYTELF-UHFFFAOYSA-N
Formula: C6H4BrClO
SMILES: Oc1ccc(Cl)cc1Br
Mol. weight [g/mol]: 207.45
CAS: 695-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.81	kJ/mol	Joback Method
hf	-108.83	kJ/mol	Joback Method
hfus	20.21	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.808		Crippen Method
mcvol	107.250	ml/mol	McGowan Method
pc	5944.56	kPa	Joback Method
tb	552.55	K	Joback Method
tc	810.23	K	Joback Method
tf	397.76	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.10	J/mol×K	552.55	Joback Method
cpg	200.12	J/mol×K	595.50	Joback Method
cpg	206.43	J/mol×K	638.44	Joback Method
cpg	212.15	J/mol×K	681.39	Joback Method
cpg	217.39	J/mol×K	724.33	Joback Method
cpg	222.25	J/mol×K	767.28	Joback Method
cpg	226.87	J/mol×K	810.23	Joback Method
dvisc	0.0011327	Pa×s	397.76	Joback Method

dvisc	0.0006305	Pa×s	423.56	Joback Method
dvisc	0.0003753	Pa×s	449.36	Joback Method
dvisc	0.0002364	Pa×s	475.15	Joback Method
dvisc	0.0001561	Pa×s	500.95	Joback Method
dvisc	0.0001074	Pa×s	526.75	Joback Method
dvisc	0.0000765	Pa×s	552.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C695965&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
mcvol: 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