2-Butanol, 3-chloro-

Other names: «beta»-Butylene chlorohydrin
3-Chloro-2-butanol
Inchi: InChI=1S/C4H9ClO/c1-3(5)4(2)6/h3-4,6H,1-2H3
InchiKey: XKEHIUIIEXXHJX-UHFFFAOYSA-N
Formula: C4H9ClO
SMILES: CC(O)C(C)Cl
Mol. weight [g/mol]: 108.57
CAS: 563-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-170.83	kJ/mol	Joback Method
hf	-304.42	kJ/mol	Joback Method
hfus	7.35	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.994		Crippen Method
mcvol	85.330	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	419.65	K	Joback Method
tc	596.68	K	Joback Method
tf	195.58	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.02	J/mol×K	419.65	Joback Method
cpg	190.75	J/mol×K	567.18	Joback Method
cpg	184.59	J/mol×K	537.67	Joback Method
cpg	178.15	J/mol×K	508.17	Joback Method
cpg	171.41	J/mol×K	478.66	Joback Method
cpg	164.37	J/mol×K	449.16	Joback Method
cpg	196.64	J/mol×K	596.68	Joback Method

dvisc	0.0002957	Pa×s	419.65	Joback Method
dvisc	0.0005484	Pa×s	382.30	Joback Method
dvisc	0.0011627	Pa×s	344.96	Joback Method
dvisc	0.0029582	Pa×s	307.62	Joback Method
dvisc	0.0097432	Pa×s	270.27	Joback Method
dvisc	0.0470292	Pa×s	232.93	Joback Method
dvisc	0.4141113	Pa×s	195.58	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=C563848&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