1-Butanol, 4-chloro-, acetate

Other names:	4-Chloro-n-butyl acetate
	4-Chlorobutyl acetate
	1-Acetoxy-4-chlorobutane
	1-Chloro-4-acetoxybutane
	4-Chlorbut-1-ylacetat
	4-Chloro-1-butanol acetate
	«delta»-Chlorobutyl acetate
	1-Butanol, 4-chloro-, 1-acetate
	NSC 53492
	NSC 54074
Inchi:	InChI=1S/C6H11ClO2/c1-6(8)9-5-3-2-4-7/h2-5H2,1H3
InchiKey:	PYLDCZJUHYVOAF-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CC(=O)OCCCCCl
Mol. weight [g/mol]:	150.60
CAS:	6962-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.568		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	450.40	K	Joback Method
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/mol×K	450.40	Joback Method
cpg	234.51	J/mol×K	481.13	Joback Method
cpg	243.77	J/mol×K	511.86	Joback Method
cpg	252.68	J/mol×K	542.58	Joback Method
cpg	261.25	J/mol×K	573.31	Joback Method
cpg	269.47	J/mol×K	604.04	Joback Method
cpg	277.34	J/mol×K	634.77	Joback Method
dvisc	0.0030315	Pa×s	259.46	Joback Method
dvisc	0.0016707	Pa×s	291.28	Joback Method
dvisc	0.0010354	Pa×s	323.11	Joback Method
dvisc	0.0006992	Pa×s	354.93	Joback Method
dvisc	0.0005036	Pa×s	386.75	Joback Method
dvisc	0.0003813	Pa×s	418.58	Joback Method
dvisc	0.0003003	Pa×s	450.40	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6962921&Units=SI

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