1-Butanol, 1-chloro, acetate

Inchi: InChI=1S/C6H11ClO2/c1-3-4-6(7)9-5(2)8/h6H,3-4H2,1-2H3
InchiKey: ZZQNKNVQFOOMEW-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CCCC(Cl)OC(C)=O
Mol. weight [g/mol]: 150.60

Physical Properties

Property code	Value	Unit	Source
gf	-248.65	kJ/mol	Joback Method
hf	-432.99	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.915		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	906.00		NIST Webbook
rinpol	912.00		NIST Webbook
ripol	1278.00		NIST Webbook
tb	449.96	K	Joback Method
tc	638.50	K	Joback Method
tf	244.46	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/mol×K	449.96	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method
cpg	244.50	J/mol×K	512.81	Joback Method
cpg	253.66	J/mol×K	544.23	Joback Method
cpg	262.46	J/mol×K	575.65	Joback Method
cpg	270.88	J/mol×K	607.08	Joback Method
cpg	278.93	J/mol×K	638.50	Joback Method

dvisc	0.0043249	Pa×s	244.46	Joback Method
dvisc	0.0020836	Pa×s	278.71	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0005117	Pa×s	381.46	Joback Method
dvisc	0.0003739	Pa×s	415.71	Joback Method
dvisc	0.0002866	Pa×s	449.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R32692&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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