1-Butanol, 2-chloro, acetate

Inchi: InChI=1S/C6H11ClO2/c1-3-6(7)4-9-5(2)8/h6H,3-4H2,1-2H3
InchiKey: BMVQKHFYSHXSBE-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CCC(Cl)COC(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	-1.46		Crippen Method
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	964.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1370.00		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

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=R32709&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
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