2-Butanol, 3-chloro-, acetate, (R*,R*)-

Inchi: InChI=1S/C6H11ClO2/c1-4(7)5(2)9-6(3)8/h4-5H,1-3H3
InchiKey: NCIUPQANRXKHMV-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CC(=O)OC(C)C(C)Cl
Mol. weight [g/mol]: 150.60
CAS: 54192-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-251.09	kJ/mol	Joback Method
hf	-438.27	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.565		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	449.52	K	Joback Method
tc	642.38	K	Joback Method
tf	229.46	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.19	J/mol×K	449.52	Joback Method
cpg	272.33	J/mol×K	610.24	Joback Method
cpg	263.70	J/mol×K	578.09	Joback Method
cpg	254.67	J/mol×K	545.95	Joback Method
cpg	245.24	J/mol×K	513.81	Joback Method
cpg	235.42	J/mol×K	481.66	Joback Method
cpg	280.57	J/mol×K	642.38	Joback Method
dvisc	0.0002735	Pa×s	449.52	Joback Method
dvisc	0.0003672	Pa×s	412.84	Joback Method

dvisc	0.0005221	Pa×s	376.17	Joback Method
dvisc	0.0008011	Pa×s	339.49	Joback Method
dvisc	0.0013635	Pa×s	302.81	Joback Method
dvisc	0.0026871	Pa×s	266.14	Joback Method
dvisc	0.0065779	Pa×s	229.46	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=C54192200&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