(+-)-3-hydroxybutyric acid, acetate

Inchi: InChI=1S/C6H10O4/c1-4(3-6(8)9)10-5(2)7/h4H,3H2,1-2H3,(H,8,9)
InchiKey: RVBYGWWJLVDBHM-UHFFFAOYSA-N
Formula: C6H10O4
SMILES: CC(=O)OC(C)CC(=O)O
Mol. weight [g/mol]: 146.14

Physical Properties

Property code	Value	Unit	Source
gf	-502.46	kJ/mol	Joback Method
hf	-682.06	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.413		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	558.58	K	Joback Method
tc	741.56	K	Joback Method
tf	325.29	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.32	J/mol×K	558.58	Joback Method
cpg	296.74	J/mol×K	711.06	Joback Method
cpg	289.78	J/mol×K	680.57	Joback Method
cpg	282.46	J/mol×K	650.07	Joback Method
cpg	274.77	J/mol×K	619.57	Joback Method
cpg	266.72	J/mol×K	589.08	Joback Method
cpg	303.34	J/mol×K	741.56	Joback Method
dvisc	0.0001238	Pa×s	558.58	Joback Method

dvisc	0.0001912	Pa×s	519.70	Joback Method
dvisc	0.0003170	Pa×s	480.82	Joback Method
dvisc	0.0005742	Pa×s	441.93	Joback Method
dvisc	0.0011665	Pa×s	403.05	Joback Method
dvisc	0.0027572	Pa×s	364.17	Joback Method
dvisc	0.0080049	Pa×s	325.29	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=U374308&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume