(+-)-2-Hydroxyoctanoic acid, acetate

Inchi: InChI=1S/C10H18O4/c1-3-4-5-6-7-9(10(12)13)14-8(2)11/h9H,3-7H2,1-2H3,(H,12,13)
InchiKey: HMUBVMKCIZTMNB-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: CCCCCCC(OC(C)=O)C(=O)O
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	-468.78	kJ/mol	Joback Method
hf	-764.62	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	70.05	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.973		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	650.10	K	Joback Method
tc	827.46	K	Joback Method
tf	370.37	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.98	J/mol×K	650.10	Joback Method
cpg	458.63	J/mol×K	679.66	Joback Method
cpg	469.73	J/mol×K	709.22	Joback Method
cpg	480.28	J/mol×K	738.78	Joback Method
cpg	490.30	J/mol×K	768.34	Joback Method
cpg	499.79	J/mol×K	797.90	Joback Method
cpg	508.75	J/mol×K	827.46	Joback Method
dvisc	0.0040995	Pa×s	370.37	Joback Method

dvisc	0.0013729	Pa×s	416.99	Joback Method
dvisc	0.0005729	Pa×s	463.61	Joback Method
dvisc	0.0002805	Pa×s	510.24	Joback Method
dvisc	0.0001548	Pa×s	556.86	Joback Method
dvisc	0.0000936	Pa×s	603.48	Joback Method
dvisc	0.0000609	Pa×s	650.10	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=U374328&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume