(Z)-3-hexenyl 3-hydroxybutanoate

Inchi: InChI=1S/C10H18O3/c1-3-4-5-6-7-13-10(12)8-9(2)11/h4-5,9,11H,3,6-8H2,1-2H3/b5-4-
InchiKey: YCRZFZCDOSZRKH-PLNGDYQASA-N
Formula: C10H18O3
SMILES: CCC=CCCOC(=O)CC(C)O
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-259.64	kJ/mol	Joback Method
hf	-534.82	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.657		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
ripol	1946.00		NIST Webbook
tb	600.39	K	Joback Method
tc	775.99	K	Joback Method
tf	315.36	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.67	J/mol×K	600.39	Joback Method
cpg	420.73	J/mol×K	629.66	Joback Method
cpg	432.25	J/mol×K	658.92	Joback Method
cpg	443.23	J/mol×K	688.19	Joback Method
cpg	453.70	J/mol×K	717.46	Joback Method
cpg	463.68	J/mol×K	746.72	Joback Method
cpg	473.16	J/mol×K	775.99	Joback Method
dvisc	0.0094331	Pa×s	315.36	Joback Method
dvisc	0.0023440	Pa×s	362.87	Joback Method

dvisc	0.0008040	Pa×s	410.37	Joback Method
dvisc	0.0003444	Pa×s	457.88	Joback Method
dvisc	0.0001730	Pa×s	505.38	Joback Method
dvisc	0.0000978	Pa×s	552.88	Joback Method
dvisc	0.0000605	Pa×s	600.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308206&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume