isobutyl 3-hydroxybutanoate

Other names: 2-Methylpropyl 3-hydroxybutanoate
Inchi: InChI=1S/C8H16O3/c1-6(2)5-11-8(10)4-7(3)9/h6-7,9H,4-5H2,1-3H3
InchiKey: DBUHENMJXAGYNE-UHFFFAOYSA-N
Formula: C8H16O3
SMILES: CC(C)COC(=O)CC(C)O
Mol. weight [g/mol]: 160.21

Physical Properties

Property code	Value	Unit	Source
gf	-359.14	kJ/mol	Joback Method
hf	-616.04	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.956		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1633.00		NIST Webbook
tb	550.03	K	Joback Method
tc	724.80	K	Joback Method
tf	282.90	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.04	J/mol×K	550.03	Joback Method
cpg	385.82	J/mol×K	695.67	Joback Method
cpg	376.36	J/mol×K	666.54	Joback Method

cpg	366.45	J/mol×K	637.42	Joback Method
cpg	356.10	J/mol×K	608.29	Joback Method
cpg	345.30	J/mol×K	579.16	Joback Method
cpg	394.85	J/mol×K	724.80	Joback Method
dvisc	0.0000978	Pa×s	550.03	Joback Method
dvisc	0.0001640	Pa×s	505.51	Joback Method
dvisc	0.0003039	Pa×s	460.99	Joback Method
dvisc	0.0006423	Pa×s	416.46	Joback Method
dvisc	0.0016241	Pa×s	371.94	Joback Method
dvisc	0.0052844	Pa×s	327.42	Joback Method
dvisc	0.0249265	Pa×s	282.90	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=R59876&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume