Propanoic acid, 2-hydroxy-, 2-methylpropyl ester

Other names: 2-Methylpropyl 2-hydroxypropanoate
Isobutyl lactate
Inchi: InChI=1S/C7H14O3/c1-5(2)4-10-7(9)6(3)8/h5-6,8H,4H2,1-3H3
InchiKey: WBPAQKQBUKYCJS-UHFFFAOYSA-N
Formula: C7H14O3
SMILES: CC(C)COC(=O)C(C)O
Mol. weight [g/mol]: 146.18
CAS: 585-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-367.56	kJ/mol	Joback Method
hf	-595.40	kJ/mol	Joback Method
hfus	13.71	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.566		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	947.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1458.00		NIST Webbook
tb	527.15	K	Joback Method
tc	703.42	K	Joback Method
tf	271.63	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.08	J/mol×K	527.15	Joback Method
cpg	336.78	J/mol×K	674.04	Joback Method
cpg	328.05	J/mol×K	644.66	Joback Method

cpg	318.91	J/mol×K	615.28	Joback Method
cpg	309.37	J/mol×K	585.91	Joback Method
cpg	299.43	J/mol×K	556.53	Joback Method
cpg	345.13	J/mol×K	703.42	Joback Method
dvisc	0.0001175	Pa×s	527.15	Joback Method
dvisc	0.0001982	Pa×s	484.56	Joback Method
dvisc	0.0003695	Pa×s	441.98	Joback Method
dvisc	0.0007868	Pa×s	399.39	Joback Method
dvisc	0.0020069	Pa×s	356.80	Joback Method
dvisc	0.0065975	Pa×s	314.22	Joback Method
dvisc	0.0314993	Pa×s	271.63	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=C585240&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume