Pentanoic acid, 4-oxo-, 2-methylpropyl ester

Other names:	iso-Butyl levulinate
	isobutyl 4-oxovalerate
Inchi:	InChI=1S/C9H16O3/c1-7(2)6-12-9(11)5-4-8(3)10/h7H,4-6H2,1-3H3
InchiKey:	WETOYPNHZMSVFZ-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CC(=O)CCC(=O)OCC(C)C
Mol. weight [g/mol]:	172.22
CAS:	3757-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-340.38	kJ/mol	Joback Method
hf	-591.75	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.555		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1183.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	535.04	K	Joback Method
tc	721.50	K	Joback Method
tf	298.28	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.82	J/mol×K	535.04	Joback Method
cpg	356.65	J/mol×K	566.12	Joback Method
cpg	368.94	J/mol×K	597.19	Joback Method
cpg	380.69	J/mol×K	628.27	Joback Method
cpg	391.90	J/mol×K	659.35	Joback Method

cpg	402.58	J/mol×K	690.42	Joback Method
cpg	412.73	J/mol×K	721.50	Joback Method
dvisc	0.0017528	Pa×s	337.74	Joback Method
dvisc	0.0035617	Pa×s	298.28	Joback Method
dvisc	0.0010005	Pa×s	377.20	Joback Method
dvisc	0.0006351	Pa×s	416.66	Joback Method
dvisc	0.0004361	Pa×s	456.12	Joback Method
dvisc	0.0003180	Pa×s	495.58	Joback Method
dvisc	0.0002429	Pa×s	535.04	Joback Method
hvapt	61.50	kJ/mol	420.50	NIST Webbook
hvapt	54.70	kJ/mol	444.00	NIST Webbook

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=C3757322&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
hvapt: Enthalpy of vaporization at a given temperature
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