iso-Amyl levulinate

Other names:	Isopentyl levulinate
	Pentanoic acid, 4-oxo-, 3-methylbutyl ester
	3-methylbutyl 4-oxopentanoate
Inchi:	InChI=1S/C10H18O3/c1-8(2)6-7-13-10(12)5-4-9(3)11/h8H,4-7H2,1-3H3
InchiKey:	NYIALINCMIXBSP-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CC(=O)CCC(=O)OCCC(C)C
Mol. weight [g/mol]:	186.25
CAS:	71172-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-331.96	kJ/mol	Joback Method
hf	-612.39	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.945		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1284.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1807.00		NIST Webbook
tb	557.92	K	Joback Method
tc	742.33	K	Joback Method
tf	309.55	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.55	J/mol×K	557.92	Joback Method
cpg	404.21	J/mol×K	588.66	Joback Method

cpg	417.28	J/mol×K	619.39	Joback Method
cpg	429.76	J/mol×K	650.13	Joback Method
cpg	441.66	J/mol×K	680.86	Joback Method
cpg	452.99	J/mol×K	711.60	Joback Method
cpg	463.74	J/mol×K	742.33	Joback Method
dvisc	0.0016605	Pa×s	350.95	Joback Method
dvisc	0.0034308	Pa×s	309.55	Joback Method
dvisc	0.0009367	Pa×s	392.34	Joback Method
dvisc	0.0005894	Pa×s	433.74	Joback Method
dvisc	0.0004021	Pa×s	475.13	Joback Method
dvisc	0.0002916	Pa×s	516.53	Joback Method
dvisc	0.0002218	Pa×s	557.92	Joback Method
hvapt	59.40	kJ/mol	462.00	NIST Webbook
hvapt	56.30	kJ/mol	461.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71172753&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
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