cis-3-hexenyl levulinate

Other names: (Z)-hex-3-enyl 4-oxovalerate
Inchi: InChI=1S/C11H18O3/c1-3-4-5-6-9-14-11(13)8-7-10(2)12/h4-5H,3,6-9H2,1-2H3/b5-4-
InchiKey: WVABNTSULPSDJL-PLNGDYQASA-N
Formula: C11H18O3
SMILES: CCC=CCCOC(=O)CCC(C)=O
Mol. weight [g/mol]: 198.26
CAS: 85554-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-240.88	kJ/mol	Joback Method
hf	-510.53	kJ/mol	Joback Method
hfus	28.83	kJ/mol	Joback Method
hvap	55.94	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.255		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
ripol	2064.00		NIST Webbook
tb	585.40	K	Joback Method
tc	771.66	K	Joback Method
tf	330.74	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.97	J/mol×K	585.40	Joback Method
cpg	432.59	J/mol×K	616.44	Joback Method
cpg	445.57	J/mol×K	647.49	Joback Method
cpg	457.91	J/mol×K	678.53	Joback Method
cpg	469.64	J/mol×K	709.57	Joback Method
cpg	480.78	J/mol×K	740.61	Joback Method
cpg	491.33	J/mol×K	771.66	Joback Method

dvisc	0.0023365	Pa×s	330.74	Joback Method
dvisc	0.0012003	Pa×s	373.18	Joback Method
dvisc	0.0007065	Pa×s	415.63	Joback Method
dvisc	0.0004588	Pa×s	458.07	Joback Method
dvisc	0.0003205	Pa×s	500.51	Joback Method
dvisc	0.0002369	Pa×s	542.96	Joback Method
dvisc	0.0001829	Pa×s	585.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85554707&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

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