(E)-2-Hexenyl formate

Inchi: InChI=1S/C7H12O2/c1-2-3-4-5-6-9-7-8/h4-5,7H,2-3,6H2,1H3/b5-4+
InchiKey: SLWYMCAVYPZTRN-SNAWJCMRSA-N
Formula: C7H12O2
SMILES: CCCC=CCOC=O
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-116.24	kJ/mol	Joback Method
hf	-288.39	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
tb	434.80	K	Joback Method
tc	614.89	K	Joback Method
tf	227.80	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.30	J/mol×K	434.80	Joback Method
cpg	234.73	J/mol×K	464.82	Joback Method
cpg	244.75	J/mol×K	494.83	Joback Method
cpg	254.34	J/mol×K	524.85	Joback Method
cpg	263.54	J/mol×K	554.86	Joback Method
cpg	272.34	J/mol×K	584.88	Joback Method
cpg	280.76	J/mol×K	614.89	Joback Method
dvisc	0.0032988	Pa×s	227.80	Joback Method

dvisc	0.0015932	Pa×s	262.30	Joback Method
dvisc	0.0009113	Pa×s	296.80	Joback Method
dvisc	0.0005856	Pa×s	331.30	Joback Method
dvisc	0.0004090	Pa×s	365.80	Joback Method
dvisc	0.0003039	Pa×s	400.30	Joback Method
dvisc	0.0002367	Pa×s	434.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R98305&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume