Propanoic acid, (E)-3-hexenyl ester

Other names: (E)-3-Hexen-1-ol, propanoate
Inchi: InChI=1S/C9H16O2/c1-3-5-6-7-8-11-9(10)4-2/h5-6H,3-4,7-8H2,1-2H3/b6-5+
InchiKey: LGTLDEUQCOJGFP-AATRIKPKSA-N
Formula: C9H16O2
SMILES: CCC=CCCOC(=O)CC
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1085.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1384.00		NIST Webbook
tb	485.77	K	Joback Method
tc	667.32	K	Joback Method
tf	258.27	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.02	J/mol×K	485.77	Joback Method
cpg	318.93	J/mol×K	516.03	Joback Method
cpg	331.30	J/mol×K	546.29	Joback Method
cpg	343.15	J/mol×K	576.54	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method
cpg	375.62	J/mol×K	667.32	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method
dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method

Sources

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=R98369&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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