Methyl (Z)-3-hexenyl carbonate

Inchi: InChI=1S/C9H16O3/c1-3-4-5-6-7-8-12-9(10)11-2/h5-6H,3-4,7-8H2,1-2H3/b6-5-
InchiKey: ZFVYNLVUYYMQBY-WAYWQWQTSA-N
Formula: C9H16O3
SMILES: CCCC=CCCOC(=O)OC
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-233.80	kJ/mol	Joback Method
hf	-488.89	kJ/mol	Joback Method
hfus	23.24	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.516		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1073.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1475.00		NIST Webbook
tb	508.19	K	Joback Method
tc	688.91	K	Joback Method
tf	280.50	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.50	J/mol×K	508.19	Joback Method
cpg	343.19	J/mol×K	538.31	Joback Method
cpg	355.40	J/mol×K	568.43	Joback Method
cpg	367.12	J/mol×K	598.55	Joback Method
cpg	378.36	J/mol×K	628.67	Joback Method
cpg	389.12	J/mol×K	658.79	Joback Method
cpg	399.42	J/mol×K	688.91	Joback Method

dvisc	0.0022388	Pa×s	280.50	Joback Method
dvisc	0.0011228	Pa×s	318.45	Joback Method
dvisc	0.0006522	Pa×s	356.40	Joback Method
dvisc	0.0004206	Pa×s	394.35	Joback Method
dvisc	0.0002930	Pa×s	432.29	Joback Method
dvisc	0.0002163	Pa×s	470.24	Joback Method
dvisc	0.0001672	Pa×s	508.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410067&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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