5-Hexenoic acid, methyl ester

Other names:	Methyl 5-hexenoate
	Methyl ester of 5-hexenoic acid
Inchi:	InChI=1S/C7H12O2/c1-3-4-5-6-7(8)9-2/h3H,1,4-6H2,2H3
InchiKey:	ASKDFGVMJZMYEM-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CCCCC(=O)OC
Mol. weight [g/mol]:	128.17
CAS:	2396-80-7

Physical Properties

Property code	Value	Unit	Source
gf	-138.02	kJ/mol	Joback Method
hf	-307.18	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	39.66	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	894.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	894.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1224.00		NIST Webbook
ripol	1223.00		NIST Webbook
tb	432.53	K	Joback Method
tc	612.55	K	Joback Method
tf	239.05	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.85	J/mol×K	432.53	Joback Method
cpg	233.32	J/mol×K	462.53	Joback Method
cpg	243.41	J/mol×K	492.54	Joback Method
cpg	253.12	J/mol×K	522.54	Joback Method
cpg	262.44	J/mol×K	552.54	Joback Method
cpg	271.40	J/mol×K	582.54	Joback Method
cpg	279.98	J/mol×K	612.55	Joback Method
dvisc	0.0028577	Pa×s	239.05	Joback Method
dvisc	0.0015177	Pa×s	271.30	Joback Method
dvisc	0.0009221	Pa×s	303.54	Joback Method
dvisc	0.0006165	Pa×s	335.79	Joback Method
dvisc	0.0004423	Pa×s	368.04	Joback Method
dvisc	0.0003347	Pa×s	400.28	Joback Method
dvisc	0.0002641	Pa×s	432.53	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396807&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
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