2-Hexenoic acid, methyl ester, (E)-

Other names: Methyl (2E)-2-hexenoate
Methyl (E)-2-hexenoate
methyl (E)-hex-2-enoate
Inchi: InChI=1S/C7H12O2/c1-3-4-5-6-7(8)9-2/h5-6H,3-4H2,1-2H3/b6-5+
InchiKey: GFUGBRNILVVWIE-AATRIKPKSA-N
Formula: C7H12O2
SMILES: CCCC=CC(=O)OC
Mol. weight [g/mol]: 128.17
CAS: 13894-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-145.64	kJ/mol	Joback Method
hf	-315.39	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1305.00		NIST Webbook
tb	440.01	K	Joback Method
tc	625.03	K	Joback Method
tf	235.73	K	Joback Method

vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.68	J/mol×K	440.01	Joback Method
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	253.64	J/mol×K	532.52	Joback Method
cpg	243.76	J/mol×K	501.68	Joback Method
cpg	233.44	J/mol×K	470.85	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0002208	Pa×s	440.01	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0029377	Pa×s	235.73	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=C13894638&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