methyl (E)-4-hexenoate

Inchi: InChI=1S/C7H12O2/c1-3-4-5-6-7(8)9-2/h3-4H,5-6H2,1-2H3/b4-3+
InchiKey: MEZYCNMPBPQTLK-ONEGZZNKSA-N
Formula: C7H12O2
SMILES: CC=CCCC(=O)OC
Mol. weight [g/mol]: 128.17

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
ripol	1237.00		NIST Webbook
ripol	1237.00		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	233.44	J/mol×K	470.85	Joback Method
cpg	243.76	J/mol×K	501.68	Joback Method
cpg	253.64	J/mol×K	532.52	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0029377	Pa×s	235.73	Joback Method

dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0002208	Pa×s	440.01	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=R319078&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume