4-Pentenoic acid ethyl ester

Other names:	Ethyl 4-pentenoate
	Ethyl pent-4-enoate
	4-Ethoxycarbonylbut-1-ene
	ethyl pent-4-en-1-oate
Inchi:	InChI=1S/C7H12O2/c1-3-5-6-7(8)9-4-2/h3H,1,4-6H2,2H3
InchiKey:	PTVSRINJXWDIKP-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CCCC(=O)OCC
Mol. weight [g/mol]:	128.17
CAS:	1968-40-7

Physical Properties

Property code	Value	Unit	Source
chl	-4038.00 ± 2.10	kJ/mol	NIST Webbook
gf	-138.02	kJ/mol	Joback Method
hf	-385.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-431.00 ± 2.00	kJ/mol	NIST Webbook
hfus	15.39	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
hvap	46.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
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
hvapt	38.00	kJ/mol	293.00	NIST Webbook

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=C1968407&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume