3-Hexenoic acid, ethyl ester

Other names: Ethyl 3-hexenoate
Ethyl hex-3-enoate
Inchi: InChI=1S/C8H14O2/c1-3-5-6-7-8(9)10-4-2/h5-6H,3-4,7H2,1-2H3/b6-5+
InchiKey: VTSFIPHRNAESED-AATRIKPKSA-N
Formula: C8H14O2
SMILES: CCC=CCC(=O)OCC
Mol. weight [g/mol]: 142.20
CAS: 2396-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-137.22	kJ/mol	Joback Method
hf	-336.03	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1003.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1290.00		NIST Webbook
tb	462.89	K	Joback Method
tc	646.21	K	Joback Method
tf	247.00	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.30	J/mol×K	462.89	Joback Method
cpg	275.19	J/mol×K	493.44	Joback Method
cpg	286.60	J/mol×K	524.00	Joback Method
cpg	297.52	J/mol×K	554.55	Joback Method
cpg	307.96	J/mol×K	585.10	Joback Method
cpg	317.95	J/mol×K	615.66	Joback Method
cpg	327.49	J/mol×K	646.21	Joback Method
dvisc	0.0030324	Pa×s	247.00	Joback Method
dvisc	0.0014687	Pa×s	282.98	Joback Method
dvisc	0.0008378	Pa×s	318.96	Joback Method
dvisc	0.0005355	Pa×s	354.94	Joback Method
dvisc	0.0003717	Pa×s	390.93	Joback Method
dvisc	0.0002744	Pa×s	426.91	Joback Method
dvisc	0.0002123	Pa×s	462.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	1.60	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396830&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume