ethyl 5-hexenoate

Other names: ethyl 5-hexenoate
Inchi: InChI=1S/C8H14O2/c1-3-5-6-7-8(9)10-4-2/h3H,1,4-7H2,2H3
InchiKey: RJLJOXJZWMGEFD-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: C=CCCCC(=O)OCC
Mol. weight [g/mol]: 142.20
CAS: 500027-11-2

Physical Properties

Property code	Value	Unit	Source
af	0.4597		Cheméo Relay (1.0)
gf	-129.60	kJ/mol	Joback Method
hf	-420.91	kJ/mol	Cheméo Relay (1.0)
hfus	17.98	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-1.83		Cheméo Relay (1.0)
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	435.00 ± 3.00	K	NIST Webbook
tc	620.57	K	Cheméo Relay (1.0)
tf	203.98	K	Cheméo Relay (1.0)
vc	0.463	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.07	J/mol×K	455.41	Joback Method
cpg	274.71	J/mol×K	485.17	Joback Method
cpg	285.90	J/mol×K	514.93	Joback Method
cpg	296.66	J/mol×K	544.69	Joback Method
cpg	306.99	J/mol×K	574.46	Joback Method
cpg	316.89	J/mol×K	604.22	Joback Method

cpg	326.37	J/mol×K	633.98	Joback Method
dvisc	0.0029783	Pa×s	250.32	Joback Method
dvisc	0.0015454	Pa×s	284.50	Joback Method
dvisc	0.0009231	Pa×s	318.68	Joback Method
dvisc	0.0006093	Pa×s	352.87	Joback Method
dvisc	0.0004328	Pa×s	387.05	Joback Method
dvisc	0.0003249	Pa×s	421.23	Joback Method
dvisc	0.0002547	Pa×s	455.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500027112&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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