10-Undecenoic acid, ethyl ester

Other names:	Ethyl 10-hendecenoate
	Ethyl 10-undecenoate
	Ethyl undecenoate
	Ethyl undecylenate
	Undecenoic acid, ethyl ester
	ethyl undec-10-enoate
Inchi:	InChI=1S/C13H24O2/c1-3-5-6-7-8-9-10-11-12-13(14)15-4-2/h3H,1,4-12H2,2H3
InchiKey:	FXNFFCMITPHEIT-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	C=CCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	212.33
CAS:	692-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-87.50	kJ/mol	Joback Method
hf	-431.02	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1469.00		NIST Webbook
tb	537.70	K	NIST Webbook
tc	741.25	K	Joback Method
tf	306.67	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.50	J/mol×K	741.25	Joback Method
cpg	494.21	J/mol×K	569.81	Joback Method

cpg	510.03	J/mol×K	598.38	Joback Method
cpg	525.18	J/mol×K	626.96	Joback Method
cpg	539.69	J/mol×K	655.53	Joback Method
cpg	553.58	J/mol×K	684.10	Joback Method
cpg	566.84	J/mol×K	712.68	Joback Method
dvisc	0.0001759	Pa×s	569.81	Joback Method
dvisc	0.0027987	Pa×s	306.67	Joback Method
dvisc	0.0013224	Pa×s	350.53	Joback Method
dvisc	0.0007382	Pa×s	394.38	Joback Method
dvisc	0.0004631	Pa×s	438.24	Joback Method
dvisc	0.0003162	Pa×s	482.10	Joback Method
dvisc	0.0002301	Pa×s	525.95	Joback Method
hvapt	77.40	kJ/mol	468.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	531.70	K	101.00	NIST Webbook
tbrp	404.70	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55477e+01
Coeff. B	-4.88633e+03
Coeff. C	-9.06170e+01
Temperature range (K), min.	410.82
Temperature range (K), max.	567.97

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=C692864&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor pressure
rinpol:	Non-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