Undecanoic acid, ethyl ester

Other names:	Ethyl n-undecanoate
	Ethyl undecanoate
	Ethyl undecylate
	n-Undecanoic acid ethyl ester
Inchi:	InChI=1S/C13H26O2/c1-3-5-6-7-8-9-10-11-12-13(14)15-4-2/h3-12H2,1-2H3
InchiKey:	IAFQYUQIAOWKSB-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	214.34
CAS:	627-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-634.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-705.40 ± 1.20	kJ/mol	NIST Webbook
hfus	36.10	kJ/mol	Thermal properties of Ethyl Undecanoate and Ethyl Tridecanoate by Adiabatic Calorimetry
hvap	72.00 ± 1.00	kJ/mol	NIST Webbook
hvap	71.40	kJ/mol	NIST Webbook
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook

rinpol	1491.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1495.40		NIST Webbook
rinpol	1495.40		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1477.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	573.13	K	Joback Method
tc	741.92	K	Joback Method
tf	308.43	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method
cpg	531.11	J/mol×K	601.26	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method

cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0001702	Pa×s	573.13	Joback Method
hfust	36.16	kJ/mol	259.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63515e+01
Coeff. B	-5.12005e+03
Coeff. C	-9.12700e+01
Temperature range (K), min.	410.00
Temperature range (K), max.	555.04

Sources

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
Thermal properties of Ethyl Undecanoate and Ethyl Tridecanoate by Adiabatic Calorimetry:	https://www.doi.org/10.1021/je050065n

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=C627907&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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor 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

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