Ethyl tridecanoate

Other names:	Tridecanoic acid ethyl ester
	n-Tridecanoic acid ethyl ester
	tridecanoic acid, ethyl ester
Inchi:	InChI=1S/C15H30O2/c1-3-5-6-7-8-9-10-11-12-13-14-15(16)17-4-2/h3-14H2,1-2H3
InchiKey:	QJYYMNOTJXIOBP-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	242.40
CAS:	28267-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-158.50	kJ/mol	Joback Method
hf	-597.73	kJ/mol	Joback Method
hfus	40.70	kJ/mol	Thermal properties of Ethyl Undecanoate and Ethyl Tridecanoate by Adiabatic Calorimetry
hvap	58.14	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1678.00		NIST Webbook

rinpol	1677.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	618.89	K	Joback Method
tc	786.41	K	Joback Method
tf	330.97	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.65	J/mol×K	786.41	Joback Method
cpg	700.70	J/mol×K	758.49	Joback Method
cpg	686.10	J/mol×K	730.57	Joback Method
cpg	670.81	J/mol×K	702.65	Joback Method
cpg	654.83	J/mol×K	674.73	Joback Method
cpg	638.14	J/mol×K	646.81	Joback Method
cpg	620.74	J/mol×K	618.89	Joback Method
dvisc	0.0025922	Pa×s	330.97	Joback Method
dvisc	0.0001371	Pa×s	618.89	Joback Method
dvisc	0.0001822	Pa×s	570.90	Joback Method
dvisc	0.0002549	Pa×s	522.92	Joback Method
dvisc	0.0003819	Pa×s	474.93	Joback Method
dvisc	0.0006264	Pa×s	426.94	Joback Method
dvisc	0.0011647	Pa×s	378.96	Joback Method
hfust	40.70	kJ/mol	272.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	395.20	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56938e+01
Coeff. B	-5.10061e+03
Coeff. C	-9.78450e+01
Temperature range (K), min.	428.92
Temperature range (K), max.	589.12

Sources

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=C28267290&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
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