Eicosanoic acid, ethyl ester

Other names:	Arachidic acid, ethyl ester
	Ethyl arachidate
	Ethyl eicosanoate
	Ethyl icosanoate
	ethyl arachate
Inchi:	InChI=1S/C22H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24-4-2
InchiKey:	YBKSMWBLSBAFBQ-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	340.58
CAS:	18281-05-5

Physical Properties

Property code	Value	Unit	Source
chs	-13895.00 ± 1.00	kJ/mol	NIST Webbook
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2394.20		NIST Webbook
rinpol	2373.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2394.20		NIST Webbook
rinpol	2379.00		NIST Webbook
rinpol	2383.00		NIST Webbook
rinpol	2379.00		NIST Webbook
rinpol	2378.00		NIST Webbook
ripol	2660.00		NIST Webbook
ripol	2649.00		NIST Webbook
ripol	2670.00		NIST Webbook
ripol	2657.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2662.00		NIST Webbook

ripol	2649.00		NIST Webbook
ripol	2649.00		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	314.52 ± 1.00	K	NIST Webbook
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.01	J/mol×K	779.05	Joback Method
cpg	1051.60	J/mol×K	808.49	Joback Method
cpg	1071.17	J/mol×K	837.93	Joback Method
cpg	1089.74	J/mol×K	867.37	Joback Method
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1139.78	J/mol×K	955.69	Joback Method
dvisc	0.0036714	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0049733	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0045070	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0040577	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0056573	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0033373	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0030462	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0027799	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0025690	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023716	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0021961	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0020395	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hfust	68.62	kJ/mol	315.00	NIST Webbook
hsubt	171.50	kJ/mol	310.00	NIST Webbook
hvapt	113.70	kJ/mol	389.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	569.20	K	13.30	NIST Webbook
tbrp	459.70	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24916e+01
Coeff. B	-9.10717e+03
Coeff. C	-1.39962e+02
Temperature range (K), min.	550.12
Temperature range (K), max.	670.06

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel: https://www.doi.org/10.1021/je1012235

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=C18281055&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

Legend

chs: Standard solid enthalpy of combustion

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
hsubt:	Enthalpy of sublimation at a given temperature
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
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