Eicosanoic acid, methyl ester

Other names:	Arachidic acid methyl ester
	Kemester 2050
	Methyl arachidate
	Methyl arachisate
	Methyl aracidate
	Methyl eicosanoate
	Methyl eicosenate
	methyl icosanoate
Inchi:	InChI=1S/C21H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h3
InchiKey:	QGBRLVONZXHAKJ-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	326.56
CAS:	1120-28-1

Physical Properties

Property code	Value	Unit	Source
chs	-13263.00 ± 0.40	kJ/mol	NIST Webbook
gf	-107.98	kJ/mol	Joback Method
hf	-721.57	kJ/mol	Joback Method
hfus	78.79	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	120.90 ± 2.50	kJ/mol	NIST Webbook
hvap	116.40 ± 1.50	kJ/mol	NIST Webbook
hvap	116.20	kJ/mol	NIST Webbook
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	378.87		NIST Webbook
rinpol	2297.80		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2300.20		NIST Webbook
rinpol	2301.40		NIST Webbook

rinpol	2302.70	NIST Webbook
rinpol	2312.00	NIST Webbook
rinpol	2314.00	NIST Webbook
rinpol	2314.00	NIST Webbook
rinpol	2296.70	NIST Webbook
rinpol	2339.00	NIST Webbook
rinpol	2310.00	NIST Webbook
rinpol	2310.00	NIST Webbook
rinpol	2311.59	NIST Webbook
rinpol	2302.00	NIST Webbook
rinpol	2318.00	NIST Webbook
rinpol	2332.00	NIST Webbook
rinpol	2311.00	NIST Webbook
rinpol	2311.00	NIST Webbook
rinpol	2317.00	NIST Webbook
rinpol	2311.00	NIST Webbook
rinpol	2329.00	NIST Webbook
rinpol	2305.00	NIST Webbook
rinpol	2333.00	NIST Webbook
rinpol	2309.00	NIST Webbook
rinpol	2313.00	NIST Webbook
rinpol	2307.00	NIST Webbook
rinpol	2307.00	NIST Webbook
rinpol	2312.00	NIST Webbook
rinpol	2324.00	NIST Webbook
rinpol	2329.00	NIST Webbook
rinpol	376.90	NIST Webbook
rinpol	380.64	NIST Webbook
rinpol	390.60	NIST Webbook
rinpol	390.60	NIST Webbook
rinpol	379.61	NIST Webbook
rinpol	2295.60	NIST Webbook
rinpol	378.87	NIST Webbook
rinpol	378.87	NIST Webbook
rinpol	2332.00	NIST Webbook
rinpol	376.90	NIST Webbook
rinpol	2335.00	NIST Webbook
rinpol	378.87	NIST Webbook
ripol	2617.00	NIST Webbook
ripol	2638.00	NIST Webbook
ripol	2640.00	NIST Webbook
ripol	2638.00	NIST Webbook
ripol	2617.00	NIST Webbook
ripol	2646.00	NIST Webbook

tb	756.17	K	Joback Method
tc	929.77	K	Joback Method
tf	398.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.32	J/mol×K	756.17	Joback Method
cpg	989.43	J/mol×K	785.10	Joback Method
cpg	1008.57	J/mol×K	814.04	Joback Method
cpg	1026.77	J/mol×K	842.97	Joback Method
cpg	1044.06	J/mol×K	871.90	Joback Method
cpg	1060.46	J/mol×K	900.83	Joback Method
cpg	1075.99	J/mol×K	929.77	Joback Method
dvisc	0.0019591	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0043226	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0038888	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0035170	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0031964	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0029177	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0026745	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0048319	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0022726	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0021066	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0024612	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hfust	74.30	kJ/mol	319.20	NIST Webbook
hfust	73.70	kJ/mol	319.20	NIST Webbook
hfust	73.70	kJ/mol	319.20	NIST Webbook
hsubt	191.00 ± 10.00	kJ/mol	314.50	NIST Webbook
hvapt	116.00	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography

hvapt	111.10	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure
hvapt	109.20	kJ/mol	350.00	NIST Webbook
hvapt	97.80 ± 0.20	kJ/mol	406.00	NIST Webbook
hvapt	76.90	kJ/mol	498.00	NIST Webbook
hvapt	92.40	kJ/mol	495.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.70	K	1.30	NIST Webbook
tbrp	461.20	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.12669e+01
Coeff. B	-8.38143e+03
Coeff. C	-1.34290e+02
Temperature range (K), min.	533.80
Temperature range (K), max.	659.59

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyl Octanoate to Methyl Eicosanoate between 5 K and 350 K:	https://www.doi.org/10.1021/je0499364
Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel:	https://www.doi.org/10.1021/je1012235
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
the vaporization enthaplies and vapor pressures of a series of unsaturated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120281&Units=SI

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