Tetracosanoic acid, methyl ester

Other names:	24:0, Me ester
	Lignoceric acid methyl ester
	Methyl lignocerate
	Methyl tetracosanoate
Inchi:	InChI=1S/C25H50O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey:	XUDJZDNUVZHSKZ-UHFFFAOYSA-N
Formula:	C25H50O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	382.66
CAS:	2442-49-1

Physical Properties

Property code	Value	Unit	Source
gf	-74.30	kJ/mol	Joback Method
hf	-804.13	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.762		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2713.00		NIST Webbook
rinpol	2710.00		NIST Webbook
rinpol	2715.00		NIST Webbook
rinpol	2729.90		NIST Webbook
rinpol	2714.00		NIST Webbook
rinpol	2731.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2712.67		NIST Webbook
rinpol	2737.00		NIST Webbook
rinpol	2731.30		NIST Webbook
rinpol	2716.00		NIST Webbook
rinpol	2687.00		NIST Webbook
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook

rinpol	2725.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	450.20		NIST Webbook
rinpol	450.30		NIST Webbook
rinpol	450.20		NIST Webbook
rinpol	2715.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2725.00		NIST Webbook
ripol	3053.00		NIST Webbook
ripol	3024.00		NIST Webbook
tb	847.69	K	Joback Method
tc	1038.15	K	Joback Method
tf	443.67	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.77	J/mol×K	847.69	Joback Method
cpg	1243.05	J/mol×K	879.43	Joback Method
cpg	1264.07	J/mol×K	911.18	Joback Method
cpg	1283.89	J/mol×K	942.92	Joback Method
cpg	1302.54	J/mol×K	974.66	Joback Method
cpg	1320.07	J/mol×K	1006.41	Joback Method
cpg	1336.53	J/mol×K	1038.15	Joback Method
dvisc	0.0027066	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0046279	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0041894	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0051392	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0034797	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0031895	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0029327	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0038102	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hfust	90.00	kJ/mol	331.20	NIST Webbook
hvapt	135.70	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography
hvapt	136.60 ± 2.50	kJ/mol	512.50	NIST Webbook
hvapt	146.20	kJ/mol	437.00	NIST Webbook
hvapt	100.80	kJ/mol	509.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	505.20	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54233e+01
Coeff. B	-6.75201e+03
Coeff. C	-1.59102e+02
Temperature range (K), min.	605.20
Temperature range (K), max.	826.84

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
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=C2442491&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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