13-Docosenoic acid, methyl ester, (Z)-

Other names:	Erucic acid methyl ester
	Methyl 13-docosenoate-, cis-
	Methyl cis-13-docosenoate
	brassidic acid, methyl ester
	cis-13-Docosenoic acid, methyl ester
	erucic acid, methyl ester
	methyl (Z)-13-docosenoate
	methyl (Z)-docos-13-enoate
	methyl erucate
Inchi:	InChI=1S/C23H44O2/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:	ZYNDJIBBPLNPOW-KHPPLWFESA-N
Formula:	C23H44O2
SMILES:	CCCCCCCCC=CCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	352.59
CAS:	1120-34-9

Physical Properties

Property code	Value	Unit	Source
chl	-14451.50 ± 1.50	kJ/mol	NIST Webbook
gf	-10.92	kJ/mol	Joback Method
hf	-645.63	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	123.80	kJ/mol	NIST Webbook
hvap	125.60 ± 1.20	kJ/mol	NIST Webbook
log10ws	-8.17		Crippen Method
logp	7.757		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2507.80		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2460.30		NIST Webbook
rinpol	2459.00		NIST Webbook
rinpol	2473.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2507.80		NIST Webbook
rinpol	2460.30		NIST Webbook

ripol	2878.00		NIST Webbook
ripol	2844.00		NIST Webbook
tb	806.09	K	Joback Method
tc	988.24	K	Joback Method
tf	416.05	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.83	J/mol×K	806.09	Joback Method
cpg	1089.32	J/mol×K	836.45	Joback Method
cpg	1108.77	J/mol×K	866.81	Joback Method
cpg	1127.22	J/mol×K	897.16	Joback Method
cpg	1144.72	J/mol×K	927.52	Joback Method
cpg	1161.30	J/mol×K	957.88	Joback Method
cpg	1177.00	J/mol×K	988.24	Joback Method
dvisc	0.0069171	Pa×s	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0149430	Pa×s	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0125560	Pa×s	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0106570	Pa×s	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0091414	Pa×s	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0079069	Pa×s	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0180870	Pa×s	278.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0059575	Pa×s	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0054021	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0047602	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0043306	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0039100	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0035480	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0032344	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0029609	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0027070	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0025097	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023223	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hvapt	125.60	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography
hvapt	93.50	kJ/mol	498.00	NIST Webbook

Sources

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=C1120349&Units=SI
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

Legend

chl:	Standard liquid 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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume