

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

Other names:	Erucic acid methyl ester Methyl 13-docosenoate-, cis- Methyl cis-13-docosenoate brassicidic 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	125.60 ± 1.20	kJ/mol	NIST Webbook
hvap	123.80	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	2460.30		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2507.80		NIST Webbook
rinpol	2473.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2507.80		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2459.00		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/molxK	806.09	Joback Method
cpg	1089.32	J/molxK	836.45	Joback Method
cpg	1108.77	J/molxK	866.81	Joback Method
cpg	1127.22	J/molxK	897.16	Joback Method
cpg	1144.72	J/molxK	927.52	Joback Method
cpg	1161.30	J/molxK	957.88	Joback Method
cpg	1177.00	J/molxK	988.24	Joback Method
dvisc	0.0069171	Paxs	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0149430	Paxs	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0125560	Paxs	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0106570	Paxs	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

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

dvisc	0.0032344	Paxs	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0029609	Paxs	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0027070	Paxs	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0025097	Paxs	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023223	Paxs	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 enthalpies and vapor pressures of a series of unstaured fatty acid methyl esters by correlation gas chromatography
hvapt	93.50	kJ/mol	498.00	NIST Webbook

## Sources

the vaporization enthalpies and vapor pressures of a series of unstaured fatty acid methyl esters by correlation gas chromatography

McGowan Method:

NIST Webbook:

Crippen Method:

<https://www.doi.org/10.1016/j.tca.2007.02.008>

<https://www.doi.org/10.1021/jc1012235>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120349&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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