cis-11-Eicosenoic acid, methyl ester

Other names:	(Z)-Methyl eicosa-11-enoate
	11-Eicosenoic acid, methyl ester, (Z)-
	Methyl (Z)-11-eicosenoate
	cis-Methyl 11-eicosenoate
	methyl cis-11-eicosenoate
	methyl cis-icos-11-enoate
Inchi:	InChI=1S/C21H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h1
InchiKey:	RBKMRGOHCLRTLZ-KHPPLWFESA-N
Formula:	C21H40O2
SMILES:	CCCCCCCCC=CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	324.54
CAS:	2390-09-2

Physical Properties

Property code	Value	Unit	Source
chl	-13190.00	kJ/mol	NIST Webbook
gf	-27.76	kJ/mol	Joback Method
hf	-604.35	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	115.80 ± 0.70	kJ/mol	NIST Webbook
log10ws	-7.33		Crippen Method
logp	6.977		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2309.50		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	760.33	K	Joback Method
tc	936.69	K	Joback Method
tf	393.51	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.56	J/mol×K	936.69	Joback Method
cpg	1018.40	J/mol×K	877.90	Joback Method
cpg	1001.56	J/mol×K	848.51	Joback Method
cpg	983.86	J/mol×K	819.12	Joback Method
cpg	965.24	J/mol×K	789.72	Joback Method
cpg	945.68	J/mol×K	760.33	Joback Method
cpg	1034.38	J/mol×K	907.29	Joback Method
dvisc	0.0025461	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0045289	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0040624	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0036649	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0033231	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0030278	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0027709	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0050803	Pa×s	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0023484	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0021736	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0020186	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0018807	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0017576	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0057379	Pa×s	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0065284	Pa×s	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	

dvisc	0.0074879	Pa×s	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0086667	Pa×s	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0101310	Pa×s	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0119750	Pa×s	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0143400	Pa×s	278.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
hvapt	115.80	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography	

Sources

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

the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methylesters by correlation gas chromatography: https://www.doi.org/10.1016/j.tca.2007.02.008

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

     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=C2390092&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume