Ethyl 9,12,15-octadecatrienoate

Other names: 9,12,14-octadecatrienoic acid, ethyl ester

9,12,15-Octadecatrienoic acid, ethyl ester

Ethyl 9«alpha»-linolenate

ethyl linolenate

linolinic acid, ethyl ester

Inchi: InChI=1S/C20H34O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h5-6,

InchiKey: JYYFMIOPGOFNPK-AGRJPVHOSA-N

Formula: C20H34O2

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCC

Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	124.26	kJ/mol	Joback Method
hf	-349.27	kJ/mol	Joback Method
hfus	50.95	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.139		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2148.00		NIST Webbook
ripol	2594.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	745.77	K	Joback Method
tc	927.85	K	Joback Method
tf	372.08	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.59	J/mol×K	745.77	Joback Method
cpg	856.73	J/mol×K	776.12	Joback Method
cpg	874.01	J/mol×K	806.46	Joback Method
cpg	890.45	J/mol×K	836.81	Joback Method
cpg	906.13	J/mol×K	867.15	Joback Method
cpg	921.08	J/mol×K	897.50	Joback Method
cpg	935.36	J/mol×K	927.85	Joback Method
dvisc	0.0032578	Pa×s	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0055379	Pa×s	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0049210	Pa×s	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0044014	Pa×s	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0039606	Pa×s	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0035831	Pa×s	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0062820	Pa×s	278.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0029750	Pa×s	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0027281	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0025114	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0023204	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0021511	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0020004	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0018658	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0017450	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	

dvisc	0.0016362	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0015382	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0014491	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0013684	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0012950	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	

Sources

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

Densities and Viscosities of Minority   https://www.doi.org/10.1021/je1012235
Fatty Acid Methyl and Ethyl Esters
Present in Biodiesel:
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=U336774&Units=SI

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

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
hvap:	Enthalpy of vaporization at standard conditions
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