9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-

Other names: Linolenic acid, ethyl ester
Ethyl cis,cis,cis-9,12,15-octadecatrienoate
Ethyl linolenate
Ethyl «alpha»-linolenate
Ethyl (Z,Z,Z)-9,12,15-octadecatrienoate
9,12,15-Octadecatrienoic acid, ethyl ester, (9Z,12Z,15Z)-
ethyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate

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

CAS: 1191-41-9

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	2165.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2145.00		NIST Webbook

rinpol	2169.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2145.00		NIST Webbook
ripol	2596.00		NIST Webbook
ripol	2591.00		NIST Webbook
ripol	2579.00		NIST Webbook
ripol	2542.00		NIST Webbook
ripol	2555.00		NIST Webbook
ripol	2596.00		NIST Webbook
ripol	2596.00		NIST Webbook
ripol	2621.00		NIST Webbook
ripol	2621.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2578.00		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	0.0013631	Pa×s	372.08	Joback Method
dvisc	0.0005220	Pa×s	434.36	Joback Method
dvisc	0.0002543	Pa×s	496.64	Joback Method
dvisc	0.0001454	Pa×s	558.92	Joback Method

dvisc	0.0000930	Pa×s	621.21	Joback Method
dvisc	0.0000646	Pa×s	683.49	Joback Method
dvisc	0.0000476	Pa×s	745.77	Joback Method
hvapt	72.70	kJ/mol	469.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	0.10	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C1191419&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
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
tbrp: Boiling point at reduced pressure

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