(E)-9-Octadecenoic acid ethyl ester

Other names:	9-Octadecenoic acid, ethyl ester, (E)-
	Ethyl 9-octadecenoate, (E)-
	Ethyl (9E)-9-octadecenoate
	Elaidic acid, ethyl ester
	Ethyl elaidate
	trans-9-Octadecenoic acid, ethyl ester
Inchi:	InChI=1S/C20H38O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h11-1
InchiKey:	LVGKNOAMLMIIKO-VAWYXSNFSA-N
Formula:	C20H38O2
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	310.51
CAS:	6114-18-7

Physical Properties

Property code	Value	Unit	Source
chl	-12528.00 ± 12.00	kJ/mol	NIST Webbook
gf	-36.18	kJ/mol	Joback Method
hf	-583.71	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.587		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2174.20		NIST Webbook
ripol	2476.00		NIST Webbook
tb	737.45	K	Joback Method
tc	911.93	K	Joback Method
tf	382.24	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	885.45	J/mol×K	737.45	Joback Method
cpg	904.58	J/mol×K	766.53	Joback Method
cpg	922.81	J/mol×K	795.61	Joback Method
cpg	940.17	J/mol×K	824.69	Joback Method
cpg	956.69	J/mol×K	853.77	Joback Method
cpg	972.40	J/mol×K	882.85	Joback Method
cpg	987.32	J/mol×K	911.93	Joback Method
dvisc	0.0015546	Pa×s	382.24	Joback Method
dvisc	0.0006381	Pa×s	441.44	Joback Method
dvisc	0.0003233	Pa×s	500.64	Joback Method
dvisc	0.0001891	Pa×s	559.84	Joback Method
dvisc	0.0001226	Pa×s	619.05	Joback Method
dvisc	0.0000857	Pa×s	678.25	Joback Method
dvisc	0.0000635	Pa×s	737.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	2.00	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=C6114187&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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