9-Octadecenoic acid, ethyl ester

Other names: Ethyl 9-octadecenoate
Ethyl octadec-9-enoate
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-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 310.51
CAS: 6512-99-8

Physical Properties

Property code	Value	Unit	Source
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	2150.00		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
ripol	2469.00		NIST Webbook
ripol	2510.00		NIST Webbook
ripol	2477.00		NIST Webbook
ripol	2466.00		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	972.40	J/mol×K	882.85	Joback Method
cpg	956.69	J/mol×K	853.77	Joback Method
cpg	940.17	J/mol×K	824.69	Joback Method
cpg	922.81	J/mol×K	795.61	Joback Method
cpg	904.58	J/mol×K	766.53	Joback Method
cpg	987.32	J/mol×K	911.93	Joback Method
dvisc	0.0000635	Pa×s	737.45	Joback Method
dvisc	0.0000857	Pa×s	678.25	Joback Method
dvisc	0.0001226	Pa×s	619.05	Joback Method
dvisc	0.0001891	Pa×s	559.84	Joback Method
dvisc	0.0003233	Pa×s	500.64	Joback Method
dvisc	0.0006381	Pa×s	441.44	Joback Method
dvisc	0.0015546	Pa×s	382.24	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C6512998&Units=SI

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