9,12-Octadecadienoic acid, ethyl ester

Other names: Ethyl-9,12-octadecadienoate
Ethyl octadec-9,12-dienoate
Ethyl octa-9,12-decadienoate
Inchi: InChI=1S/C20H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h8-9,
InchiKey: FMMOOAYVCKXGMF-MVKOLZDDSA-N
Formula: C20H36O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 308.50
CAS: 7619-08-1

Physical Properties

Property code	Value	Unit	Source
gf	44.04	kJ/mol	Joback Method
hf	-466.49	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.363		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
ripol	2560.00		NIST Webbook
ripol	2515.00		NIST Webbook
ripol	2527.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2527.00		NIST Webbook
tb	741.61	K	Joback Method
tc	919.70	K	Joback Method
tf	377.16	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.13	J/mol×K	741.61	Joback Method

cpg	880.77	J/mol×K	771.29	Joback Method
cpg	898.51	J/mol×K	800.97	Joback Method
cpg	915.41	J/mol×K	830.65	Joback Method
cpg	931.49	J/mol×K	860.34	Joback Method
cpg	946.80	J/mol×K	890.02	Joback Method
cpg	961.38	J/mol×K	919.70	Joback Method
dvisc	0.0014552	Pa×s	377.16	Joback Method
dvisc	0.0005772	Pa×s	437.90	Joback Method
dvisc	0.0002868	Pa×s	498.64	Joback Method
dvisc	0.0001659	Pa×s	559.38	Joback Method
dvisc	0.0001068	Pa×s	620.13	Joback Method
dvisc	0.0000744	Pa×s	680.87	Joback Method
dvisc	0.0000550	Pa×s	741.61	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7619081&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume