Heptadecanoic acid, ethyl ester

Other names:	Ethyl heptadecanoate
	Ethyl n-heptadecanoate
Inchi:	InChI=1S/C19H38O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-4-2/h3-18H2
InchiKey:	KNXMUFRWYNVISA-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	298.50
CAS:	14010-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-124.82	kJ/mol	Joback Method
hf	-680.29	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.421		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2074.00		NIST Webbook
rinpol	2089.00		NIST Webbook
ripol	2359.00		NIST Webbook
ripol	2348.00		NIST Webbook
ripol	2342.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2349.00		NIST Webbook
ripol	2355.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2349.00		NIST Webbook
ripol	2370.00		NIST Webbook

ripol	2357.00		NIST Webbook
ripol	2383.00		NIST Webbook
tb	710.41	K	Joback Method
tc	879.90	K	Joback Method
tf	376.05	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.34	J/mol×K	879.90	Joback Method
cpg	936.27	J/mol×K	851.65	Joback Method
cpg	920.41	J/mol×K	823.40	Joback Method
cpg	903.75	J/mol×K	795.15	Joback Method
cpg	886.25	J/mol×K	766.91	Joback Method
cpg	867.91	J/mol×K	738.66	Joback Method
cpg	848.69	J/mol×K	710.41	Joback Method
dvisc	0.0018384	Pa×s	376.05	Joback Method
dvisc	0.0000838	Pa×s	710.41	Joback Method
dvisc	0.0001126	Pa×s	654.68	Joback Method
dvisc	0.0001599	Pa×s	598.96	Joback Method
dvisc	0.0002440	Pa×s	543.23	Joback Method
dvisc	0.0004101	Pa×s	487.50	Joback Method
dvisc	0.0007881	Pa×s	431.78	Joback Method
hfust	36.20	kJ/mol	298.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.94072e+01
Coeff. B	-7.24324e+03
Coeff. C	-1.23282e+02
Temperature range (K), min.	502.12
Temperature range (K), max.	637.14

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C14010232&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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor 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