11-Octadecenoic acid, (E)-

Other names:	(E)-octadec-11-enoic acid
	Vaccenic acid
	trans-11-octadecenoic acid
	trans-Vaccenic acid
Inchi:	InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h8-9H,2-7,1
InchiKey:	QXJSBBXBKPUZAA-CMDGGOBGSA-N
Formula:	C18H34O2
SMILES:	CCCCCCCC=CCCCCCCCCC(=O)O
Mol. weight [g/mol]:	282.46
CAS:	693-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-84.84	kJ/mol	Joback Method
hf	-562.44	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	79.05	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.109		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
tb	761.45	K	Joback Method
tc	937.21	K	Joback Method
tf	316.65 ± 1.00	K	NIST Webbook
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.35	J/mol×K	761.45	Joback Method
cpg	827.83	J/mol×K	790.74	Joback Method
cpg	843.52	J/mol×K	820.04	Joback Method
cpg	858.48	J/mol×K	849.33	Joback Method
cpg	872.72	J/mol×K	878.62	Joback Method

cpg	886.31	J/mol×K	907.92	Joback Method
cpg	899.26	J/mol×K	937.21	Joback Method
dvisc	0.0006419	Pa×s	458.82	Joback Method
dvisc	0.0023727	Pa×s	398.29	Joback Method
dvisc	0.0002355	Pa×s	519.34	Joback Method
dvisc	0.0001065	Pa×s	579.87	Joback Method
dvisc	0.0000560	Pa×s	640.40	Joback Method
dvisc	0.0000329	Pa×s	700.92	Joback Method
dvisc	0.0000210	Pa×s	761.45	Joback Method
hfust	58.49	kJ/mol	317.00	NIST Webbook
hfust	55.62	kJ/mol	318.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52924e+01
Coeff. B	-5.81882e+03
Coeff. C	-1.25923e+02
Temperature range (K), min.	514.15
Temperature range (K), max.	709.15

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=C693721&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume