Elaidic acid

Other names:	(E)-9-octadecenoic acid
	trans-9-octadecenoic acid
	trans-«delta»
	9-Octadecenoic acid, (E)-
Inchi:	InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h9-10H,2-8,
InchiKey:	ZQPPMHVWECSIRJ-MDZDMXLPSA-N
Formula:	C18H34O2
SMILES:	CCCCCCCC/C=C/CCCCCCCC(=O)O
Mol. weight [g/mol]:	282.47
CAS:	112-79-8

Physical Properties

Property code	Value	Unit	Source
af	1.0245		Cheméo Relay (1.0)
chs	-11040.40	kJ/mol	NIST Webbook
gf	-163.01	kJ/mol	Joback Method
hf	-675.90	kJ/mol	Cheméo Relay (1.0)
hfl	-769.00	kJ/mol	NIST Webbook
hfus	52.72	kJ/mol	Joback Method
hvap	126.06	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-5.93		Cheméo Relay (1.0)
logp	6.109		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
tb	601.79	K	Cheméo Relay (1.0)
tc	809.13	K	Cheméo Relay (1.0)
tf	317.15 ± 1.00	K	NIST Webbook
tf	320.00 ± 1.00	K	NIST Webbook
tf	316.95 ± 0.50	K	NIST Webbook
tf	287.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	1.005	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	61.55	kJ/mol	317.60	NIST Webbook
hfust	27.03	kJ/mol	371.20	NIST Webbook
hvapt	133.00	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
hvapt	82.30	kJ/mol	539.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	561.20	K	13.30	NIST Webbook
tbrp	507.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.30560e+01
Coeff. B	1.78462e+00
Coeff. C	-1.11180e-03
Coeff. D	2.78400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc

Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.31254e+01
Coeff. B	2.75050e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	310.31
Temperature range (K), max.	660.17

Information	Value
Property code	pvap
Equation	ln(Y) = A + B/(T + C)
Y unit	kPa
Coeff. A	2.06467e+01
Coeff. B	-1.04353e+04
Coeff. C	1.58860e+01
Reference	Stull, 1947
Comment	Coefficents calculated by NIST from author's data.
Temperature range (K), min.	444.50
Temperature range (K), max.	635.00

Sources

Cheméo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112798&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid 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
hfl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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