9-Octadecenoic acid

Other names: (E)-9-octadecenoic acid
9-octadecenoic acid, (E)-
Oleic acid
elaidic acid
trans-9-octadecenoic acid
trans-«delta»
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: CCCCCCCCC=CCCCCCCCC(=O)O
Mol. weight [g/mol]: 282.46
CAS: 2027-47-6

Physical Properties

Property code	Value	Unit	Source
chl	-11128.00	kJ/mol	NIST Webbook
chl	-11127.10	kJ/mol	NIST Webbook
chs	-11040.40	kJ/mol	NIST Webbook
gf	-84.84	kJ/mol	Joback Method
hf	-562.44	kJ/mol	Joback Method
hfl	-769.00	kJ/mol	NIST Webbook
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
rinpol	2141.00		NIST Webbook
rinpol	2143.90		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	761.45	K	Joback Method
tc	937.21	K	Joback Method
tf	316.95 ± 0.50	K	NIST Webbook
tf	317.15 ± 1.00	K	NIST Webbook
tf	320.00 ± 1.00	K	NIST Webbook
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.31	J/mol×K	907.92	Joback Method
cpg	899.26	J/mol×K	937.21	Joback Method
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
dvisc	0.0000329	Pa×s	700.92	Joback Method
dvisc	0.0000210	Pa×s	761.45	Joback Method
dvisc	0.0023727	Pa×s	398.29	Joback Method
dvisc	0.0006419	Pa×s	458.82	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
hfust	27.03	kJ/mol	371.20	NIST Webbook
hfust	61.55	kJ/mol	317.60	NIST Webbook
hvapt	82.30	kJ/mol	539.50	NIST Webbook
hvapt	133.00	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of some Fatty Acids:	https://www.doi.org/10.1021/je300902c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume