9,12,15-Octadecatrienoic acid, (Z,Z,Z)-

Other names:	(Z,Z,Z)-9,12,15-Octadecatrienoic acid .alpha.-linolenic acid ALPHA-LINOLENIC ACID CIS,CIS,CIS-9,12,15-OCTADECATRIENOIC ACID Industrene 120 LINOLENIC ACID all-cis-9,12,15-octadecatrienoic acid «alpha»-Linolenic acid
Inchi:	InChI=1S/C18H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h3-4,6-7,9-1
InchiKey:	DTOSIQBPPRVQHS-PDBXOOCHSA-N
Formula:	C18H30O2
SMILES:	CCC=CCC=CCC=CCCCCCCCC(=O)O
Mol. weight [g/mol]:	278.43
CAS:	463-40-1

Physical Properties

Property code	Value	Unit	Source
gf	75.60	kJ/mol	Joback Method
hf	-328.00	kJ/mol	Joback Method
hfl	-508.80	kJ/mol	NIST Webbook
hfus	48.67	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.661		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2122.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2158.90		NIST Webbook
rinpol	2113.00		NIST Webbook

rinpol	2099.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2115.00		NIST Webbook
ripol	3292.00		NIST Webbook
ripol	3250.00		NIST Webbook
ripol	3292.00		NIST Webbook
ripol	3300.00		NIST Webbook
ripol	3250.00		NIST Webbook
ripol	3292.00		NIST Webbook
tb	769.77	K	Joback Method
tc	951.83	K	Joback Method
tf	388.13	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.47	J/mol×K	769.77	Joback Method
cpg	777.83	J/mol×K	800.11	Joback Method
cpg	792.49	J/mol×K	830.46	Joback Method
cpg	806.48	J/mol×K	860.80	Joback Method
cpg	819.88	J/mol×K	891.14	Joback Method
cpg	832.74	J/mol×K	921.49	Joback Method
cpg	845.11	J/mol×K	951.83	Joback Method
dvisc	0.0000155	Pa×s	769.77	Joback Method
dvisc	0.0005488	Pa×s	451.74	Joback Method
dvisc	0.0001891	Pa×s	515.34	Joback Method
dvisc	0.0022584	Pa×s	388.13	Joback Method
dvisc	0.0000423	Pa×s	642.56	Joback Method
dvisc	0.0000245	Pa×s	706.16	Joback Method
dvisc	0.0000823	Pa×s	578.95	Joback Method
hvapt	136.90	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

kvisc	0.0000155	m2/s	293.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
kvisc	0.0000124	m2/s	303.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
kvisc	0.0000089	m2/s	313.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
kvisc	0.0000073	m2/s	323.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
kvisc	0.0000060	m2/s	333.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds
kvisc	0.0000051	m2/s	343.15	Group Contribution Model for Predicting Viscosity of Fatty Compounds

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	504.20	K	0.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Activity coefficient at infinite dilution measurements for organic solutes (polar and non-polar) in fatty compounds. Part II: C18 fatty acids:	https://www.doi.org/10.1016/j.jct.2012.12.009
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/je300902c
Phase equilibrium measurements of ternary systems formed by linoleic and linolenic acids in carbon dioxide/ethanol mixtures:	https://www.doi.org/10.1016/j.jct.2009.05.012
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C463401&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=983
Group Contribution Model for Predicting Viscosity of Fatty Compounds:	https://www.doi.org/10.1021/je600552b

Legend

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
kvisc:	Kinematic viscosity
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
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

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