

Nonadecanoic acid

Other names:	n-Nonadecanoic acid nonadecylic acid
Inchi:	InChI=1S/C19H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21/h2-18H2
InchiKey:	ISYWECDZWTKFF-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	298.50
CAS:	646-30-0

Physical Properties

Property code	Value	Unit	Source
chl	-11923.40 ± 2.30	kJ/mol	NIST Webbook
gf	-156.64	kJ/mol	Joback Method
hf	-700.30	kJ/mol	Joback Method
hfus	50.65	kJ/mol	Joback Method
hsub	192.00	kJ/mol	NIST Webbook
hvap	81.31	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.723		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	780.17	K	Joback Method
tc	956.58	K	Joback Method
tf	340.70 ± 2.00	K	NIST Webbook
tf	372.40 ± 0.30	K	NIST Webbook
tf	338.80 ± 1.00	K	NIST Webbook
tf	372.40 ± 0.40	K	NIST Webbook
tf	341.45 ± 0.40	K	NIST Webbook
tf	341.33 ± 0.05	K	NIST Webbook
tt	341.23 ± 0.02	K	NIST Webbook
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.68	J/mol×K	927.18	Joback Method
cpg	988.34	J/mol×K	956.58	Joback Method
cpg	945.14	J/mol×K	868.38	Joback Method
cpg	929.20	J/mol×K	838.97	Joback Method
cpg	912.43	J/mol×K	809.57	Joback Method
cpg	894.79	J/mol×K	780.17	Joback Method
cpg	960.29	J/mol×K	897.78	Joback Method
cps	525.35	J/mol×K	298.15	NIST Webbook
dvisc	0.0000204	Pa×s	780.17	Joback Method
dvisc	0.0005734	Pa×s	475.56	Joback Method
dvisc	0.0002172	Pa×s	536.48	Joback Method
dvisc	0.0000534	Pa×s	658.33	Joback Method
dvisc	0.0000317	Pa×s	719.25	Joback Method
dvisc	0.0020135	Pa×s	414.64	Joback Method
dvisc	0.0001003	Pa×s	597.40	Joback Method
hfust	9.76	kJ/mol	338.00	NIST Webbook
hfust	57.62	kJ/mol	341.20	NIST Webbook
hfust	57.00	kJ/mol	340.40	NIST Webbook
hfust	57.62	kJ/mol	341.20	NIST Webbook
hsubt	143.60	kJ/mol	306.50	NIST Webbook
hvapt	121.80	kJ/mol	382.50	NIST Webbook
hvapt	94.40	kJ/mol	585.00	NIST Webbook
hvapt	138.00	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
sfust	168.87	J/mol×K	341.20	NIST Webbook
sfust	28.87	J/mol×K	338.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	570.70	K	13.30	NIST Webbook
tbrp	502.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.80999e+01
Coeff. B	-7.05633e+03
Coeff. C	-1.30371e+02
Temperature range (K), min.	526.52
Temperature range (K), max.	682.15

Sources

KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=953
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646300&Units=SI
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.chemed.com/doc/models/crippen_log10ws
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids:	https://www.doi.org/10.1021/jc300902c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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