Heptadecanoic acid

Other names:	Margaric acid
	Margarinic acid
	N-MARGARIC ACID
	Normal-heptadecanoic acid
	n-Heptadecanoic acid
	n-Heptadecoic acid
	n-Heptadecylic acid
Inchi:	InChI=1S/C17H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h2-16H2,1H3,(
InchiKey:	KEMQGTRYUADPNZ-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	270.45
CAS:	506-12-7

Physical Properties

Property code	Value	Unit	Source
chl	-10624.40 ± 1.70	kJ/mol	NIST Webbook
gf	-173.48	kJ/mol	Joback Method
hf	-659.02	kJ/mol	Joback Method
hfus	45.47	kJ/mol	Joback Method
hvap	76.86	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.942		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1393.90 ± 85.00	kPa	NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2022.00		NIST Webbook
rinpol	2038.00		NIST Webbook

rinpol	351.50		NIST Webbook
rinpol	351.70		NIST Webbook
rinpol	337.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2086.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2044.00		NIST Webbook
rinpol	2039.00		NIST Webbook
ripol	3027.00		NIST Webbook
ripol	2974.00		NIST Webbook
ripol	3027.00		NIST Webbook
ripol	2975.00		NIST Webbook
ripol	2979.00		NIST Webbook
ripol	2975.00		NIST Webbook
ripol	2981.00		NIST Webbook
ripol	2974.00		NIST Webbook
ripol	2968.00		NIST Webbook
tb	734.41	K	Joback Method
tc	795.08 ± 3.00	K	NIST Webbook
tf	334.40 ± 0.05	K	NIST Webbook
tf	333.00 ± 3.00	K	NIST Webbook
tf	332.80 ± 2.00	K	NIST Webbook
tf	323.40 ± 2.00	K	NIST Webbook
tf	333.00 ± 0.40	K	NIST Webbook
tf	333.00 ± 0.30	K	NIST Webbook
tf	333.00 ± 0.30	K	NIST Webbook
tf	334.15 ± 0.35	K	NIST Webbook
tt	334.25 ± 0.02	K	NIST Webbook
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.09	J/mol×K	734.41	Joback Method
cpg	793.61	J/mol×K	762.84	Joback Method
cpg	809.36	J/mol×K	791.27	Joback Method
cpg	824.37	J/mol×K	819.70	Joback Method
cpg	838.67	J/mol×K	848.13	Joback Method
cpg	852.28	J/mol×K	876.56	Joback Method

cpg	865.23	J/mol×K	905.00	Joback Method
cps	475.74	J/mol×K	298.15	NIST Webbook
dvisc	0.0008408	Pa×s	449.15	Joback Method
dvisc	0.0003178	Pa×s	506.20	Joback Method
dvisc	0.0001463	Pa×s	563.25	Joback Method
dvisc	0.0000777	Pa×s	620.31	Joback Method
dvisc	0.0000459	Pa×s	677.36	Joback Method
dvisc	0.0029520	Pa×s	392.10	Joback Method
dvisc	0.0000294	Pa×s	734.41	Joback Method
hfust	51.33	kJ/mol	334.30	NIST Webbook
hfust	51.90	kJ/mol	333.00	NIST Webbook
hfust	46.50	kJ/mol	333.50	NIST Webbook
hfust	51.33	kJ/mol	334.30	NIST Webbook
hfust	7.44	kJ/mol	329.20	NIST Webbook
hsubt	151.00	kJ/mol	291.00	NIST Webbook
hsubt	168.00	kJ/mol	303.50	NIST Webbook
hvapt	127.30	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
hvapt	100.70	kJ/mol	543.00	NIST Webbook
hvapt	112.70 ± 2.00	kJ/mol	369.50	NIST Webbook
sfust	22.59	J/mol×K	329.20	NIST Webbook
sfust	153.55	J/mol×K	334.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	500.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61967e+01
Coeff. B	-5.93946e+03
Coeff. C	-1.18222e+02

Temperature range (K), min.	491.56
Temperature range (K), max.	663.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.21328e+02
Coeff. B	-3.99733e+04
Coeff. C	-7.20295e+01
Coeff. D	2.74316e-05
Temperature range (K), min.	449.15
Temperature range (K), max.	637.15

Sources

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=C506127&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=951
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

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
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
ripol:	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