Eicosanoic acid

Other names:	ARACHIC ACID
	Arachidic acid
	Arachidic acid (synthetic)
	Icosanoic acid
	N-EICOSANOIC ACID
Inchi:	InChI=1S/C20H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h2-19
InchiKey:	VKOBVWXKNCXXDE-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	312.53
CAS:	506-30-9

Physical Properties

Property code	Value	Unit	Source
chl	-12574.20 ± 1.50	kJ/mol	NIST Webbook
gf	-148.22	kJ/mol	Joback Method
hf	-720.94	kJ/mol	Joback Method
hfus	53.24	kJ/mol	Joback Method
hvap	83.54	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.113		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
pt	2.00e-06 ± 1.07e-06	kPa	NIST Webbook
rinpol	377.80		NIST Webbook
rinpol	2365.30		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2365.30		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2366.00		NIST Webbook
rinpol	377.80		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	803.05	K	Joback Method
tc	983.47	K	Joback Method

tf	348.40 ± 0.05	K	NIST Webbook
tt	347.25 ± 0.60	K	NIST Webbook
tt	348.23 ± 0.02	K	NIST Webbook
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.42	J/mol×K	953.40	Joback Method
cpg	1007.04	J/mol×K	893.26	Joback Method
cpg	990.60	J/mol×K	863.19	Joback Method
cpg	973.29	J/mol×K	833.12	Joback Method
cpg	955.05	J/mol×K	803.05	Joback Method
cpg	1051.45	J/mol×K	983.47	Joback Method
cpg	1022.64	J/mol×K	923.33	Joback Method
cps	545.14	J/mol×K	298.15	NIST Webbook
dvisc	0.0004736	Pa×s	488.77	Joback Method
dvisc	0.0001796	Pa×s	551.62	Joback Method
dvisc	0.0000830	Pa×s	614.48	Joback Method
dvisc	0.0000443	Pa×s	677.34	Joback Method
dvisc	0.0000263	Pa×s	740.19	Joback Method
dvisc	0.0016627	Pa×s	425.91	Joback Method
dvisc	0.0000169	Pa×s	803.05	Joback Method
hfust	69.20	kJ/mol	348.20	NIST Webbook
hfust	69.20	kJ/mol	348.20	NIST Webbook
hfust	71.60	kJ/mol	347.80	NIST Webbook
hsubt	200.00 ± 7.50	kJ/mol	336.80	NIST Webbook
hsubt	199.60 ± 7.50	kJ/mol	341.50	NIST Webbook
hsubt	148.40	kJ/mol	314.00	NIST Webbook
hvapt	125.50	kJ/mol	392.00	NIST Webbook
hvapt	114.50	kJ/mol	573.50	NIST Webbook
hvapt	143.70	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.85579e+01
Coeff. B	-7.38557e+03
Coeff. C	-1.34680e+02
Temperature range (K), min.	538.92
Temperature range (K), max.	692.23

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=954
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C506309&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pt:	Triple Point Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume