Eicosane

Other names: icosane
n-Eicosane
n-Icosane
Inchi: InChI=1S/C20H42/c1-3-5-7-9-11-13-15-17-19-20-18-16-14-12-10-8-6-4-2/h3-20H2,1-2H3
InchiKey: CBFCDTFDPHXCNY-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 282.55
CAS: 112-95-8

Physical Properties

Property code	Value	Unit	Source
af	0.9070		KDB
chl	-13316.40 ± 2.80	kJ/mol	NIST Webbook
gf	117.40	kJ/mol	KDB
hf	-456.10	kJ/mol	KDB
hf	-455.80 ± 3.10	kJ/mol	NIST Webbook
hfl	-556.50 ± 3.10	kJ/mol	NIST Webbook
hfus	69.03	kJ/mol	Solid liquid equilibria and purity determination for binary n-alkane + naphthalene systems
hsub	170.40	kJ/mol	NIST Webbook
hvap	101.10 ± 2.00	kJ/mol	NIST Webbook
hvap	101.80	kJ/mol	NIST Webbook
hvap	103.50	kJ/mol	NIST Webbook
hvap	102.80 ± 2.20	kJ/mol	NIST Webbook
hvap	102.60 ± 1.00	kJ/mol	NIST Webbook
hvap	100.80	kJ/mol	NIST Webbook
log10ws	-8.17		Aqueous Solubility Prediction Method
log10ws	-8.17		Estimated Solubility Method
logp	8.048		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1070.00	kPa	KDB
pc	1100.00 ± 200.00	kPa	NIST Webbook
pc	1070.00 ± 40.00	kPa	NIST Webbook

rinpol	345.20		NIST Webbook
rinpol	345.20		NIST Webbook
rinpol	331.90		NIST Webbook
rinpol	333.60		NIST Webbook
rinpol	327.63		NIST Webbook
ss	558.60	J/mol×K	NIST Webbook
tb	582.90 ± 5.00	K	NIST Webbook
tb	616.20	K	NIST Webbook
tb	616.00	K	KDB
tc	767.50 ± 3.00	K	NIST Webbook
tc	769.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tc	768.00	K	KDB
tc	768.00 ± 8.00	K	NIST Webbook
tf	308.18	K	Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1- octadecanol, or + 1-eicosanol mixtures
tf	308.10	K	Determination of thermophysical properties of cyclopentane hydrate using a stirred calorimetric cell
tf	310.05	K	Solid-liquid equilibria of indole binary systems
tf	309.77	K	Aqueous Solubility Prediction Method
tf	309.51	K	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
tf	309.90	K	KDB
tt	309.20	K	Solubilities of Some Long-Chain n-Alkanes in Dipropyl Ether, Dibutyl Ether, 1-Chlorobutane, and 1-Chlorooctane as Functions of Temperature
tt	309.70 ± 0.20	K	NIST Webbook
tt	309.64 ± 0.01	K	NIST Webbook
vc	1.155	m3/kmol	Joback Method
zra	0.23		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.72	J/mol×K	737.19	Joback Method
cpg	861.41	J/mol×K	683.73	Joback Method
cpg	840.49	J/mol×K	657.00	Joback Method
cpg	919.16	J/mol×K	763.92	Joback Method
cpg	936.82	J/mol×K	790.65	Joback Method
cpg	953.72	J/mol×K	817.38	Joback Method
cpg	881.48	J/mol×K	710.46	Joback Method
cpl	664.00	J/mol×K	325.00	NIST Webbook
cps	602.50	J/mol×K	279.10	NIST Webbook
dvisc	0.0012516	Pa×s	372.13	Joback Method
dvisc	0.0000972	Pa×s	657.00	Joback Method
dvisc	0.0001334	Pa×s	600.03	Joback Method
dvisc	0.0036329	Pa×s	315.16	Joback Method
dvisc	0.0003143	Pa×s	486.08	Joback Method
dvisc	0.0005722	Pa×s	429.11	Joback Method
dvisc	0.0001958	Pa×s	543.05	Joback Method
hfust	67.80	kJ/mol	308.80	NIST Webbook
hfust	61.48	kJ/mol	309.70	NIST Webbook
hfust	67.80	kJ/mol	309.70	NIST Webbook
hfust	68.10	kJ/mol	309.70	NIST Webbook
hfust	69.80	kJ/mol	310.20	NIST Webbook
hfust	69.87	kJ/mol	309.75	NIST Webbook
hfust	67.80	kJ/mol	308.80	NIST Webbook
hfust	70.90	kJ/mol	308.50	NIST Webbook
hfust	69.00	kJ/mol	309.60	NIST Webbook
hsubt	179.50 ± 2.00	kJ/mol	367.00	NIST Webbook
hsubt	172.80 ± 3.00	kJ/mol	305.00	NIST Webbook
hvapt	68.30	kJ/mol	506.50	NIST Webbook
hvapt	57.49	kJ/mol	617.00	KDB
hvapt	103.90	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure

hvapt	71.10	kJ/mol	574.00	NIST Webbook
hvapt	99.50 ± 1.10	kJ/mol	343.00	NIST Webbook
hvapt	89.60	kJ/mol	411.50	NIST Webbook
hvapt	93.30	kJ/mol	362.00	NIST Webbook
hvapt	80.80	kJ/mol	506.50	NIST Webbook
hvapt	79.00	kJ/mol	407.50	NIST Webbook
hvapt	110.00 ± 2.00	kJ/mol	367.50	NIST Webbook
hvapt	78.00	kJ/mol	508.00	NIST Webbook
hvapt	80.78 ± 0.07	kJ/mol	440.00	NIST Webbook
psub	5.94e-06	kPa	307.86	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
psub	3.30e-06	kPa	304.59	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
psub	1.73e-06	kPa	302.37	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
psub	4.59e-06	kPa	306.79	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
pvap	1.46e-05	kPa	313.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	4.91e-05	kPa	323.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone

pvap	4.87e-05	kPa	323.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	1.47e-04	kPa	333.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	4.90e-05	kPa	323.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	4.64e-05	kPa	323.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	3.87e-04	kPa	343.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
pvap	4.88e-05	kPa	323.15	The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone
rhol	775.00	kg/m3	313.00	KDB
sfust	229.80	J/mol×K	308.50	NIST Webbook
sfust	225.60	J/mol×K	309.75	NIST Webbook

sfust	219.60	J/mol×K	308.80	NIST Webbook
sfust	198.50	J/mol×K	309.70	NIST Webbook
srf	0.03	N/m	323.15	Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane
srf	0.03	N/m	333.15	Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane
srf	0.03	N/m	343.15	Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane
srf	0.03	N/m	313.15	Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane
srf	0.03	N/m	323.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.20	K	4.00	NIST Webbook
tfp	318.15	K	33520.00	High pressure solid solid and solid liquid transition data for long chain alkanes
tfp	323.15	K	55080.00	High pressure solid solid and solid liquid transition data for long chain alkanes
tfp	328.15	K	76800.00	High pressure solid solid and solid liquid transition data for long chain alkanes

tfp	333.15	K	99090.00	High pressure solid solid and solid liquid transition data for long chain alkanes
tfp	344.91	K	150000.00	High pressure solid solid and solid liquid transition data for long chain alkanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47405e+01
Coeff. B	-5.08531e+03
Coeff. C	-1.14538e+02
Temperature range (K), min.	466.39
Temperature range (K), max.	653.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.25740e+02
Coeff. B	-1.58831e+04
Coeff. C	-1.50009e+01
Coeff. D	2.63411e-06
Temperature range (K), min.	309.59
Temperature range (K), max.	767.04

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid

323.65	7300.00	771.0
323.65	14900.00	777.0
323.65	21400.00	784.0
323.65	27400.00	787.0
323.65	34200.00	789.0
422.85	7400.00	711.0
422.85	14300.00	719.0
422.85	20600.00	723.0
422.85	27900.00	730.0
422.85	34600.00	735.0
422.85	54200.00	748.0
422.85	81600.00	765.0
422.85	109200.00	781.0
422.85	136100.00	792.0
422.85	169500.00	806.0
422.85	203100.00	818.0
422.85	235500.00	829.0
422.85	260000.00	837.0
522.55	16400.00	661.0
522.55	28300.00	676.0
522.55	41900.00	691.0
522.55	55500.00	706.0
522.55	69600.00	719.0
522.55	82500.00	727.0
522.55	109200.00	744.0
522.55	138200.00	763.0
522.55	173100.00	777.0
522.55	204700.00	791.0
522.55	239800.00	805.0
522.55	258000.00	810.0

Reference *https://www.doi.org/10.1016/j.fluid.2011.08.020*

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
325.80	6700.00	0.0031840
325.80	6700.00	0.0031930
325.80	14400.00	0.0035110
325.80	14400.00	0.0035280
325.80	21300.00	0.0038280

325.80	22300.00	0.0039080
325.80	28700.00	0.0042500
325.80	35500.00	0.0046420
429.30	5500.00	0.0008370
429.30	7400.00	0.0008580
429.30	21800.00	0.0010290
429.30	41800.00	0.0012620
429.30	63000.00	0.0014980
429.30	63000.00	0.0015230
429.30	83000.00	0.0017770
429.30	103700.00	0.0020430
429.30	125000.00	0.0023510
429.30	144500.00	0.0026310
429.30	144700.00	0.0026380
429.30	167900.00	0.0029880
429.30	187900.00	0.0033210
429.30	208900.00	0.0036850
429.30	228600.00	0.0040400
429.30	243100.00	0.0043270
533.80	6200.00	0.0003460
533.80	22900.00	0.0004250
533.80	43300.00	0.0005410
533.80	43500.00	0.0005410
533.80	63200.00	0.0006470
533.80	84300.00	0.0007500
533.80	104400.00	0.0008610
533.80	125000.00	0.0009770
533.80	146100.00	0.0010970
533.80	165900.00	0.0011990
533.80	187300.00	0.0013410
533.80	208200.00	0.0014440
533.80	228800.00	0.0015560

Reference *https://www.doi.org/10.1016/j.jct.2014.01.008*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Interfacial Tension Measurement and Calculation of (Carbon Dioxide + n-Alkane) Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00159
Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane:	https://www.doi.org/10.1021/je050024r
Measurements and modeling of high-temperature, high-pressure density for binary mixtures of propane with n-decane and propane with n-eicosane:	https://www.doi.org/10.1016/j.jct.2014.12.015

High pressure solid solid and solid liquid transition data for long chain alkanes:	https://www.doi.org/10.1016/j.jct.2008.07.017
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Bubble Pressure Measurement and Prediction for n-Hexadecane and n-Eicosane + Cyclohexane, Methylcyclohexane, and Ethylcyclohexane Binary Mixtures from 303.15 to 393.15 K:	https://www.doi.org/10.1021/acs.jced.8b00125
Solid-liquid equilibria and purity determination for binary n-alkane + naphthalene systems:	https://www.doi.org/10.1016/j.tca.2006.03.011
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique: The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444
Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C26:	https://www.doi.org/10.1021/je800534x
Influence of a-Olefin Concentration and Length on the High-Pressure Phase Behavior of (a-Olefin + n-Hexane + LLDPE) Systems:	https://www.doi.org/10.1021/acs.jced.9b00224
Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures:	https://www.doi.org/10.1016/j.fluid.2017.03.012
Solubilities of Some Long-Chain n-Alkanes in Dipropyl Ether, Dibutyl Ether, 1-Chlorobutane, and 1-Chlorooctane as Functions of Temperature:	https://www.doi.org/10.1021/je030206q
KDB:	https://www.cheric.org/files/research/kdb/mol/mol20.mol
Solid-liquid equilibria of indole binary systems:	https://www.doi.org/10.1016/j.tca.2016.10.003
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112958&Units=SI
Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique:	https://www.doi.org/10.1016/j.fluid.2014.07.017
Determination of thermophysical properties of cyclopentane hydrate using a stirred calorimetric cell:	https://www.doi.org/10.1016/j.jct.2018.05.023
Phase behaviour in the vicinity of the three-phase solid liquid vapour line in asymmetric nonpolar systems at high pressures:	https://www.doi.org/10.1016/j.fluid.2005.11.031
Viscosity of n-hexadecane, n-octadecane and n-eicosane at pressures up to 243 MPa and temperatures up to 534 K:	https://www.doi.org/10.1016/j.jct.2014.01.008
Article Previous Article Next Article Articles ASAP Use of Equations of State and Coarse Grained Simulations to Complement Experiments: Describing the Interfacial Properties of Carbon Dioxide + Decane and Carbon Dioxide + Eicosane Mixtures:	https://www.doi.org/10.1021/je5000764
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=20
Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure:	https://www.doi.org/10.1016/j.fluid.2006.02.001
Experimental measurements and equation of state modeling of liquid densities for long-chain n-alkanes at pressures to 265 MPa and temperatures to 523 K:	https://www.doi.org/10.1016/j.fluid.2011.08.020
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Use of Antioxidants to Improve Vapor Pressure Measurements on Compounds with Oxidative Instability: Methyl Oleate with tert-Butylhydroquinone:	https://www.doi.org/10.1021/acs.jced.6b00821

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase 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
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature
vc:	Critical Volume
zra:	Rackett Parameter