Octacosane

Other names:	n-Octacosane
Inchi:	InChI=1S/C28H58/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28-26-24-22-20-18-16-14-12-
InchiKey:	ZYURHZPYMFLWSH-UHFFFAOYSA-N
Formula:	C28H58
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	394.76
CAS:	630-02-4

Physical Properties

Property code	Value	Unit	Source
gf	184.88	kJ/mol	Joback Method
hf	-621.25	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hsub	209.00 ± 10.00	kJ/mol	NIST Webbook
hvap	141.90	kJ/mol	NIST Webbook
hvap	150.80 ± 0.50	kJ/mol	NIST Webbook
hvap	150.70 ± 1.70	kJ/mol	NIST Webbook
hvap	152.40 ± 2.90	kJ/mol	NIST Webbook
log10ws	-11.54		Crippen Method
logp	11.169		Crippen Method
mcvol	405.380	ml/mol	McGowan Method
pc	655.44	kPa	Joback Method
rinpol	442.42		NIST Webbook
rinpol	461.80		NIST Webbook
rinpol	461.80		NIST Webbook
tb	704.80	K	NIST Webbook
tc	836.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	334.55	K	KDB

tt	330.40	K	Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C32)
tt	333.98 ± 0.70	K	NIST Webbook
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.97	J/mol×K	840.04	Joback Method
cpg	1373.48	J/mol×K	871.73	Joback Method
cpg	1397.66	J/mol×K	903.42	Joback Method
cpg	1420.59	J/mol×K	935.11	Joback Method
cpg	1442.33	J/mol×K	966.80	Joback Method
cpg	1462.92	J/mol×K	998.49	Joback Method
cpg	1482.44	J/mol×K	1030.18	Joback Method
cpl	937.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0018142	Pa×s	398.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0013609	Pa×s	423.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0006847	Pa×s	498.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering

dvisc	0.0005675	Pa×s	523.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0010252	Pa×s	448.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0008318	Pa×s	473.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0004753	Pa×s	548.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
dvisc	0.0003995	Pa×s	573.15	Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 573 K by Surface Light Scattering
hfust	64.64	kJ/mol	334.50	NIST Webbook
hfust	67.38	kJ/mol	334.20	NIST Webbook
hfust	64.64	kJ/mol	334.50	NIST Webbook
hfust	35.44	kJ/mol	331.30	NIST Webbook
hfust	63.00	kJ/mol	333.40	NIST Webbook
hsubt	195.80 ± 2.20	kJ/mol	326.00	NIST Webbook
hvapt	105.50	kJ/mol	459.50	NIST Webbook
hvapt	100.60	kJ/mol	512.50	NIST Webbook
hvapt	98.10	kJ/mol	512.50	NIST Webbook
hvapt	131.70	kJ/mol	345.00	NIST Webbook

hvapt	106.60	kJ/mol	593.00	NIST Webbook
hvapt	135.00 ± 3.00	kJ/mol	431.50	NIST Webbook
hvapt	118.50	kJ/mol	435.50	NIST Webbook
hvapt	117.40 ± 1.20	kJ/mol	375.50	NIST Webbook
hvapt	141.90	kJ/mol	298.15	Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography
hvapt	128.60	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	99.27 ± 0.06	kJ/mol	510.00	NIST Webbook
hvapt	103.10 ± 3.00	kJ/mol	494.00	NIST Webbook
hvapt	100.50	kJ/mol	535.50	NIST Webbook
psub	1.17e-08	kPa	323.05	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
psub	2.37e-08	kPa	326.15	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
psub	4.39e-08	kPa	329.02	Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28
pvap	0.43	kPa	516.89	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)

pvap	0.16	kPa	494.80	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	2.14e-06	kPa	354.01	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	1.77e-05	kPa	373.92	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	0.04	kPa	473.64	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	0.01	kPa	453.28	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)

pvap	2.93e-03	kPa	433.32	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	6.30e-04	kPa	413.50	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	6.51e-04	kPa	413.50	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	6.33e-04	kPa	413.50	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	1.26e-04	kPa	393.65	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)

pvap	1.22e-04	kPa	393.65	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	1.80e-05	kPa	373.92	A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28)
pvap	1.70	kPa	550.62	Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures
sfust	193.28	J/mol×K	334.50	NIST Webbook
sfust	106.98	J/mol×K	331.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	551.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.69575e+01
Coeff. B	-7.53939e+03
Coeff. C	-9.37360e+01
Temperature range (K), min.	546.01
Temperature range (K), max.	741.12

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.55627e+02
Coeff. B	-3.27960e+04
Coeff. C	-4.75245e+01
Coeff. D	1.44719e-05
Temperature range (K), min.	481.15
Temperature range (K), max.	704.15

Sources

Vapor and Sublimation Pressures of Three Normal Alkanes: C20, C24, and C28:	https://www.doi.org/10.1021/je800534x
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number structures, and solvent chemistry on (solubility):	https://www.doi.org/10.1016/j.fluid.2004.10.021
Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures:	https://www.doi.org/10.1021/acs.jced.8b00168
KDB:	https://www.cheric.org/files/research/kdb/mol/mol28.mol
NIST-Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630024&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
A Gas Saturation Apparatus for Very Low Vapor or Sublimation Pressure Measurements (10-3 Pa): Vapor-Liquid Equilibria of n-Alkanes (n-C10, n-C24, n-C28):	https://www.doi.org/10.1021/je7001122
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0301747
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=28
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid Viscosity and Surface Tension of n-Dodecane, n-Octacosane, Their Mixtures, and a Wax between 323 and 373 K by Surface Light Scattering:	https://www.doi.org/10.1021/acs.jced.7b00363
Measurement of the thermal conductivity of wax phase change materials via DSC and transient plane source methods:	https://www.doi.org/10.1016/j.tca.2014.09.022
Liquid Viscosity and Surface Tension of Binary and Ternary Mixtures Needed to Estimate the Behaviour of the Bulk Material in Applications: Surface Light Scattering:	https://www.doi.org/10.1021/acs.jced.8b01139
Thermal conductivity of heavy n-alkanes (C22 to C32):	https://www.doi.org/10.1016/j.fluid.2018.08.016

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid 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
psub:	Sublimation 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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