DOCOSANE

Other names: Normal-docosane
n-docosane
Inchi: InChI=1S/C22H46/c1-3-5-7-9-11-13-15-17-19-21-22-20-18-16-14-12-10-8-6-4-2/h3-22H2
InchiKey: HOWGUJZVBDQJKV-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.61
CAS: 629-97-0

Physical Properties

Property code	Value	Unit	Source
af	0.9367		Cheméo Relay (1.0)
gf	134.36	kJ/mol	Joback Method
hf	-505.98	kJ/mol	Cheméo Relay (1.0)
hfus	52.74	kJ/mol	Joback Method
hvap	115.60 ± 1.90	kJ/mol	NIST Webbook
hvap	111.90	kJ/mol	NIST Webbook
hvap	114.90 ± 0.30	kJ/mol	NIST Webbook
hvap	115.60	kJ/mol	NIST Webbook
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-9.22		Cheméo Relay (1.0)
logp	8.828		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	980.00	kPa	KDB
pc	1000.00 ± 200.00	kPa	NIST Webbook
pc	982.00 ± 40.00	kPa	NIST Webbook
rinpol	374.90		NIST Webbook
rinpol	374.90		NIST Webbook
rinpol	374.90		NIST Webbook
rinpol	362.61		NIST Webbook
rinpol	356.14		NIST Webbook
tb	641.80	K	NIST Webbook
tc	763.15 ± 10.00	K	NIST Webbook
tc	785.60 ± 3.00	K	NIST Webbook
tc	786.00 ± 8.00	K	NIST Webbook
tc	786.00	K	KDB

tc	787.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	317.60 ± 0.60	K	NIST Webbook
tf	317.30 ± 0.60	K	NIST Webbook
tf	317.60 ± 3.00	K	NIST Webbook
tf	317.55 ± 1.00	K	NIST Webbook
tf	317.00 ± 2.00	K	NIST Webbook
tf	317.60 ± 1.00	K	NIST Webbook
tf	317.40 ± 0.70	K	NIST Webbook
tf	315.80 ± 4.00	K	NIST Webbook
tf	317.70 ± 0.80	K	NIST Webbook
tf	313.20 ± 3.00	K	NIST Webbook
tf	317.70 ± 2.00	K	NIST Webbook
tf	317.70 ± 0.70	K	NIST Webbook
tf	317.00 ± 2.00	K	NIST Webbook
tf	317.00 ± 0.30	K	NIST Webbook
tf	317.00 ± 2.00	K	NIST Webbook
tf	317.60 ± 0.80	K	NIST Webbook
tf	317.06 ± 0.20	K	NIST Webbook
tf	317.20 ± 0.30	K	NIST Webbook
tf	314.00 ± 4.00	K	NIST Webbook
tf	317.07 ± 0.40	K	NIST Webbook
tf	318.30 ± 3.00	K	NIST Webbook
tf	316.93 ± 0.25	K	NIST Webbook
tf	317.30 ± 0.20	K	NIST Webbook
tf	316.05 ± 1.00	K	NIST Webbook
tf	316.00 ± 0.10	K	NIST Webbook
tf	316.85 ± 0.15	K	NIST Webbook
tf	316.74 ± 0.07	K	NIST Webbook
tf	317.05 ± 0.30	K	NIST Webbook
tt	315.60	K	Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C32)
tt	317.22	K	Magnetic effect on the phase transitions of n-docosane by means of a high resolution and super-sensitive DSC
tt	315.20 ± 1.00	K	NIST Webbook
vc	1.320	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.09	J/mol×K	839.25	Joback Method
cpg	1079.56	J/mol×K	866.55	Joback Method
cpg	962.02	J/mol×K	702.76	Joback Method
cpg	983.83	J/mol×K	730.06	Joback Method
cpg	1004.72	J/mol×K	757.36	Joback Method
cpg	1024.70	J/mol×K	784.66	Joback Method
cpg	1043.81	J/mol×K	811.95	Joback Method
cpl	739.00	J/mol×K	353.00	NIST Webbook
cps	563.60	J/mol×K	299.00	NIST Webbook
cps	468.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0001534	Pa×s	581.07	Joback Method
dvisc	0.0029440	Pa×s	337.70	Joback Method
dvisc	0.0010030	Pa×s	398.54	Joback Method
dvisc	0.0004545	Pa×s	459.39	Joback Method
dvisc	0.0002478	Pa×s	520.23	Joback Method
dvisc	0.0001040	Pa×s	641.92	Joback Method
dvisc	0.0000755	Pa×s	702.76	Joback Method
hfust	47.84	kJ/mol	316.10	NIST Webbook
hfust	78.50	kJ/mol	316.90	NIST Webbook
hfust	29.51	kJ/mol	315.20	NIST Webbook
hfust	47.84	kJ/mol	316.10	NIST Webbook
hfust	49.10	kJ/mol	316.60	NIST Webbook
hsubt	172.60 ± 2.00	kJ/mol	391.00	NIST Webbook
hvapt	110.00	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	111.90	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	84.30	kJ/mol	513.00	NIST Webbook
hvapt	124.00 ± 2.00	kJ/mol	391.00	NIST Webbook
hvapt	89.90	kJ/mol	424.00	NIST Webbook
hvapt	100.90	kJ/mol	407.50	NIST Webbook
hvapt	91.30	kJ/mol	536.50	NIST Webbook
sfust	151.36	J/mol×K	316.10	NIST Webbook
sfust	93.62	J/mol×K	315.20	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.28366e+02
Coeff. B	-1.54319e+04
Coeff. C	-1.57784e+01
Coeff. D	5.23129e-06
Temperature range (K), min.	431.15
Temperature range (K), max.	649.15

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=22
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
Magnetic effect on the phase transitions of n-docosane by means of a high resolution and super-sensitive DSC:	https://www.doi.org/10.1016/j.tca.2013.08.001
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=22
Cheméo Relay (1.0, beta):	
Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C32):	https://www.doi.org/10.1016/j.fluid.2018.08.016
Excess Molar Volumes for Three and Four Component Mixtures Simulating the Binary Mixture (Cyclohexane-Hexadecane):	https://www.doi.org/10.1021/acs.jced.5b00331
Examination of hydrogen-bonding interactions between dissolved solutes and alkylbenzene solvents based on Abraham model correlations derived from measured enthalpies of solvation:	https://www.doi.org/10.1016/j.tca.2014.08.024
Cheméo Relay (1.0):	
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 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
Surface tension of decane binary and ternary mixtures with eicosane, docosane and tetracosane:	https://www.doi.org/10.1021/je050024r
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629970&Units=SI

Legend

af:	Acentric Factor
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
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
ie:	Ionization energy
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume