Heptadecane

Other names:	Normal-heptadecane
	n-Heptadecane
Inchi:	InChI=1S/C17H36/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3-17H2,1-2H3
InchiKey:	NDJKXXJCMXVBJW-UHFFFAOYSA-N
Formula:	C17H36
SMILES:	CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	240.47
CAS:	629-78-7

Physical Properties

Property code	Value	Unit	Source
af	0.7700		KDB
chl	-11351.20 ± 2.20	kJ/mol	NIST Webbook
gf	92.15	kJ/mol	KDB
hf	-393.90 ± 2.40	kJ/mol	NIST Webbook
hf	-394.20	kJ/mol	KDB
hfl	-479.50 ± 2.40	kJ/mol	NIST Webbook
hfus	39.79	kJ/mol	Joback Method
hsub	125.10	kJ/mol	NIST Webbook
hvap	86.02	kJ/mol	NIST Webbook
hvap	86.00 ± 0.80	kJ/mol	NIST Webbook
hvap	86.20	kJ/mol	NIST Webbook
hvap	86.50	kJ/mol	NIST Webbook
log10ws	-6.94		Crippen Method
logp	6.878		Crippen Method
mcvol	250.390	ml/mol	McGowan Method
pc	1342.00 ± 160.00	kPa	NIST Webbook
pc	1300.00 ± 200.00	kPa	NIST Webbook
pc	1340.00	kPa	KDB
pc	1320.00 ± 40.00	kPa	NIST Webbook
rhoc	216.42 ± 48.09	kg/m3	NIST Webbook
rhoc	218.10 ± 4.81	kg/m3	NIST Webbook
rinpol	287.19		NIST Webbook
rinpol	282.99		NIST Webbook
sl	652.24	J/mol×K	NIST Webbook
tb	575.10	K	KDB
tb	561.65 ± 2.00	K	NIST Webbook

tb	563.15 ± 2.00	K	NIST Webbook
tb	561.65 ± 1.50	K	NIST Webbook
tb	574.25 ± 0.70	K	NIST Webbook
tb	575.00	K	NIST Webbook
tc	736.00 ± 3.00	K	NIST Webbook
tc	735.60	K	NIST Webbook
tc	735.90 ± 1.00	K	NIST Webbook
tc	725.30 ± 1.60	K	NIST Webbook
tc	731.10 ± 3.00	K	NIST Webbook
tc	736.00 ± 2.00	K	NIST Webbook
tc	736.00	K	KDB
tc	736.00 ± 5.00	K	NIST Webbook
tf	301.00 ± 5.00	K	NIST Webbook
tf	294.90 ± 0.30	K	NIST Webbook
tf	295.11 ± 0.02	K	NIST Webbook
tf	295.11 ± 0.02	K	NIST Webbook
tf	295.13 ± 0.01	K	NIST Webbook
tf	295.13 ± 0.01	K	NIST Webbook
tf	295.15 ± 1.00	K	NIST Webbook
tf	295.11 ± 0.06	K	NIST Webbook
tf	294.95 ± 0.50	K	NIST Webbook
tf	295.10 ± 0.10	K	NIST Webbook
tf	295.01 ± 0.15	K	NIST Webbook
tf	295.08 ± 0.20	K	NIST Webbook
tf	295.00 ± 0.20	K	NIST Webbook
tf	295.00 ± 0.20	K	NIST Webbook
tf	294.87 ± 0.20	K	NIST Webbook
tf	294.40 ± 0.50	K	NIST Webbook
tf	294.40 ± 0.20	K	NIST Webbook
tf	294.39 ± 0.20	K	NIST Webbook
tf	295.09 ± 0.20	K	NIST Webbook
tf	294.00 ± 2.00	K	NIST Webbook
tf	295.35	K	High pressure phase equilibria in methane +waxy systems 1. Methane + heptadecane
tf	296.00 ± 2.00	K	NIST Webbook
tf	296.00 ± 2.00	K	NIST Webbook
tf	295.40 ± 2.00	K	NIST Webbook
tf	295.70 ± 2.00	K	NIST Webbook
tf	295.00 ± 4.00	K	NIST Webbook
tf	295.00	K	KDB
tf	295.00 ± 2.00	K	NIST Webbook
tf	295.00 ± 3.00	K	NIST Webbook
tf	295.13 ± 0.03	K	NIST Webbook

tf	295.70 ± 2.00	K	NIST Webbook
tt	295.14 ± 0.04	K	NIST Webbook
vc	1.103	m3/kmol	NIST Webbook
vc	1.103	m3/kmol	KDB
zc	0.2415270		KDB
zra	0.23		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.92	J/mol×K	588.36	Joback Method
cpg	705.41	J/mol×K	641.24	Joback Method
cpg	723.52	J/mol×K	667.68	Joback Method
cpg	740.91	J/mol×K	694.12	Joback Method
cpg	757.59	J/mol×K	720.56	Joback Method
cpg	773.60	J/mol×K	747.00	Joback Method
cpg	686.55	J/mol×K	614.80	Joback Method
cpl	534.34	J/mol×K	298.15	NIST Webbook
dvisc	0.0001869	Pa×s	537.19	Joback Method
dvisc	0.0002719	Pa×s	486.02	Joback Method
dvisc	0.0001372	Pa×s	588.36	Joback Method
dvisc	0.0007760	Pa×s	383.69	Joback Method
dvisc	0.0016701	Pa×s	332.52	Joback Method
dvisc	0.0047502	Pa×s	281.35	Joback Method
dvisc	0.0004318	Pa×s	434.86	Joback Method
hfust	10.96	kJ/mol	284.30	NIST Webbook
hfust	40.17	kJ/mol	295.10	NIST Webbook
hfust	39.40	kJ/mol	294.70	NIST Webbook
hfust	40.17	kJ/mol	295.10	NIST Webbook
hsubt	131.00 ± 13.00	kJ/mol	290.50	NIST Webbook
hsubt	131.50 ± 4.60	kJ/mol	288.00	NIST Webbook
hvapt	52.89	kJ/mol	576.00	KDB
hvapt	71.60	kJ/mol	457.50	NIST Webbook
hvapt	62.90	kJ/mol	532.50	NIST Webbook
hvapt	91.10	kJ/mol	304.50	NIST Webbook

rfi	1.42680		318.15	Thermodynamic properties of (an ester + an alkane). XVI. Experimental HEm and V Em values and a new correlation method for (an alkyl ethanoate + an n-alkane) at 318.15 K
rfi	1.43620		293.10	Liquid liquid equilibria for n-alkanes (C12, C14, C17) + propylbenzene +NMP mixtures at temperatures between 298 and 328K
rfi	1.43620		293.10	Extraction of pentylbenzene from high molar mass alkanes (C14 and C17) by N-methyl-2-pyrrolidone
rhol	736.80	kg/m3	353.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	729.80	kg/m3	363.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa

rhol	723.00	kg/m3	373.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	743.70	kg/m3	343.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	750.45	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	757.30	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa

rhol	764.16	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	771.02	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane, or n-Heptadecane) at 0.1 MPa
rhol	778.00	kg/m3	298.00	KDB
sfust	38.56	J/mol×K	284.30	NIST Webbook
sfust	136.11	J/mol×K	295.10	NIST Webbook
srf	0.03	N/m	303.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	434.90	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46994e+01

Coeff. B	-4.66990e+03
Coeff. C	-1.12064e+02
Temperature range (K), min.	436.10
Temperature range (K), max.	609.50

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.59113e+02
Coeff. B	-2.12295e+04
Coeff. C	-3.50392e+01
Coeff. D	1.53105e-05
Temperature range (K), min.	295.13
Temperature range (K), max.	733.37

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol17.mol
Interfacial Tension Measurement and Calculation of (Carbon Dioxide + n-Alkane) Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00159
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629787&Units=SI
Liquid liquid equilibria for n-alkanes (C12, C14, C17) + propylbenzene +NMP mixtures at temperatures between 298 and 328K:	https://www.doi.org/10.1016/j.fluid.2005.01.012
Extraction of propylbenzene from its mixtures with heptadecane using 4-methyl-N-butylpyridinium tetrafluoroborate:	https://www.doi.org/10.1016/j.fluid.2011.11.008
Experiment and correlation of the equilibrium interfacial tension for paraffin + CO2 modified with ethanol:	https://www.doi.org/10.1016/j.jct.2017.08.031
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15 K:	https://www.doi.org/10.1016/j.jct.2004.12.014
Measurement and correlation of the interfacial tension for paraffin + CO2 and (CO2+N2) mixture gas at elevated pressures:	https://www.doi.org/10.1016/j.fluid.2017.02.012
Measurement of bubble point pressure in crude oils using an acoustic wave sensor:	https://www.doi.org/10.1016/j.fluid.2016.07.003
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=17
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
High pressure phase equilibria in methane +waxy systems 1. Methane + heptadecane:	https://www.doi.org/10.1016/j.fluid.2007.04.014
Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Ethylbenzene + Linear Alkanes (n-Decane, n-Dodecane, n-Tetradecane, n-Hexadecane) at 318.15 K:	https://www.doi.org/10.1021/acs.jced.6b00542
Thermodynamic properties of (an ester + an alkane). XVI. Experimental HEm and a new correlation method for (an alkyl ethanoate + an alkane):	https://www.doi.org/10.1016/j.jct.2003.11.008
JobackE Method:	https://en.wikipedia.org/wiki/Joback_method
Extraction of phenylbenzene from high molar mass alkanes (C14 and C17) by N-methyl-2-pyrrolidone:	https://www.doi.org/10.1016/j.jct.2005.06.012

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
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
zc:	Critical Compressibility
zra:	Rackett Parameter

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