Tetracontane

Other names:	n-Tetracontane
Inchi:	InChI=1S/C40H82/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-40-38-36-
InchiKey:	KUPLEGDPSCCPJI-UHFFFAOYSA-N
Formula:	C40H82
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	563.08
CAS:	4181-95-7

Physical Properties

Property code	Value	Unit	Source
gf	285.92	kJ/mol	Joback Method
hf	-868.93	kJ/mol	Joback Method
hfus	143.94	kJ/mol	Observation of multiple phase transitions in some even n-alkanes using a high resolution and super-sensitive DSC
hvap	203.50 ± 0.20	kJ/mol	NIST Webbook
log10ws	-16.57		Crippen Method
logp	15.850		Crippen Method
mcvol	574.460	ml/mol	McGowan Method
pc	390.88	kPa	Joback Method
tb	1114.60	K	Joback Method
tc	904.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	353.70 ± 4.00	K	NIST Webbook
tf	353.90 ± 1.50	K	NIST Webbook
tf	353.50 ± 4.00	K	NIST Webbook
tf	354.50 ± 1.00	K	NIST Webbook
tf	354.55 ± 0.30	K	NIST Webbook
tf	354.00 ± 3.00	K	NIST Webbook
tf	354.50 ± 1.50	K	NIST Webbook
vc	2.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2176.15	J/mol×K	1114.60	Joback Method
cpg	2363.61	J/mol×K	1428.91	Joback Method
cpg	2331.42	J/mol×K	1366.05	Joback Method
cpg	2394.55	J/mol×K	1491.78	Joback Method
cpg	2297.26	J/mol×K	1303.19	Joback Method
cpg	2260.46	J/mol×K	1240.33	Joback Method
cpg	2220.32	J/mol×K	1177.46	Joback Method
dvisc	0.0000177	Pa×s	827.58	Joback Method
dvisc	0.0000106	Pa×s	923.25	Joback Method
dvisc	0.0000070	Pa×s	1018.93	Joback Method
dvisc	0.0000050	Pa×s	1114.60	Joback Method
dvisc	0.0002420	Pa×s	540.56	Joback Method
dvisc	0.0000778	Pa×s	636.23	Joback Method
dvisc	0.0000337	Pa×s	731.91	Joback Method
hfust	143.94	kJ/mol	354.60	NIST Webbook
hfust	133.44	kJ/mol	353.20	NIST Webbook
hfust	14.02	kJ/mol	345.40	NIST Webbook
hfust	133.44	kJ/mol	353.20	NIST Webbook
hvapt	203.50	kJ/mol	298.15	Hypothetical Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even n-Alkanes from C40 to C76 at T = 298.15 K by Correlation-Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?
hvapt	132.20	kJ/mol	677.50	NIST Webbook
sfust	377.82	J/mol×K	353.20	NIST Webbook
sfust	40.58	J/mol×K	345.40	NIST Webbook

tdiff	6.73e-08	m2/s	448.57	Thermal and Mutual Diffusivity of Binary Mixtures of n-Dodecane and n-Tetracontane with Carbon Monoxide, Hydrogen, and Water from Dynamic Light Scattering (DLS)
tdiff	6.57e-08	m2/s	448.09	Thermal and Mutual Diffusivity of Binary Mixtures of n-Dodecane and n-Tetracontane with Carbon Monoxide, Hydrogen, and Water from Dynamic Light Scattering (DLS)
tdiff	6.86e-08	m2/s	473.26	Thermal and Mutual Diffusivity of Binary Mixtures of n-Dodecane and n-Tetracontane with Carbon Monoxide, Hydrogen, and Water from Dynamic Light Scattering (DLS)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43328e+01
Coeff. B	-5.51646e+03
Coeff. C	-2.33050e+02
Temperature range (K), min.	625.81
Temperature range (K), max.	844.54

Sources

Observation of multiple phase transitions in some even n-alkanes using a high resolution and super-heated DSC:	https://www.doi.org/10.1016/j.tca.2006.06.022
Phase behaviour in the vicinity of the three-phase solid-liquid vapour line in asymmetric homologa systems at high pressures:	https://www.doi.org/10.1016/j.fluid.2005.11.031
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
High pressure solid-solid and solid-liquid transition data for long chain alkanes:	https://www.doi.org/10.1016/j.jct.2008.07.017
Quantitative Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even Alkanes (n-C40 to n-C60) at 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je7005852
Thermal and Mutual Diffusivity of Binary Mixtures of n-Dodecane and n-Tetradecane with Carbon Monoxide, Hydrogen, and Water from Dynamic Light Scattering (DLS):	https://www.doi.org/10.1021/acs.jced.5b00986
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4181957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Are the Vaporization Enthalpies a Linear Function of Carbon Number?:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas 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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tdiff:	Thermal diffusivity
tf:	Normal melting (fusion) point
vc:	Critical Volume

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