Hexatriacontane

Other names: n-Hexatriacontane
Inchi: InChI=1S/C36H74/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-36-34-32-30-28-
InchiKey: YDLYQMBWCWFRAI-UHFFFAOYSA-N
Formula: C36H74
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 506.97
CAS: 630-06-8

Physical Properties

Property code	Value	Unit	Source
gf	252.24	kJ/mol	Joback Method
hf	-786.37	kJ/mol	Joback Method
hfus	102.51	kJ/mol	Observation of multiple phase transitions in some even n-alkanes using a high resolution and super-sensitive DSC
hfus	81.55	kJ/mol	Solid liquid equilibria and purity determination for binary n-alkane + naphthalene systems
hvap	182.80	kJ/mol	NIST Webbook
log10ws	-14.89		Crippen Method
logp	14.290		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	457.74	kPa	Joback Method
tb	348.88	K	KDB
tc	888.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	349.20 ± 0.60	K	NIST Webbook
tf	349.40 ± 1.00	K	NIST Webbook
tf	348.30 ± 1.00	K	NIST Webbook
tf	350.00 ± 6.00	K	NIST Webbook
tf	349.20 ± 0.60	K	NIST Webbook
tf	349.00 ± 0.05	K	NIST Webbook
tf	349.00 ± 2.00	K	NIST Webbook
tf	349.20 ± 0.50	K	NIST Webbook
tf	349.20 ± 2.00	K	NIST Webbook

tf	349.90 ± 1.00	K	NIST Webbook
tf	348.00 ± 2.00	K	NIST Webbook
tf	349.00 ± 3.00	K	NIST Webbook
tf	349.00 ± 0.60	K	NIST Webbook
tf	348.40 ± 4.00	K	NIST Webbook
tf	351.70 ± 4.00	K	NIST Webbook
tf	349.00 ± 2.00	K	NIST Webbook
tf	349.00 ± 2.00	K	NIST Webbook
tf	349.90 ± 1.00	K	NIST Webbook
tf	348.88 ± 0.20	K	NIST Webbook
tf	349.10 ± 0.50	K	NIST Webbook
tf	350.00 ± 2.00	K	NIST Webbook
tf	349.00 ± 3.00	K	NIST Webbook
tf	349.10 ± 0.50	K	NIST Webbook
tf	348.70 ± 1.00	K	NIST Webbook
tf	349.00 ± 0.40	K	NIST Webbook
tf	349.05 ± 0.50	K	NIST Webbook
tf	349.20 ± 0.30	K	NIST Webbook
tf	348.88	K	KDB
vc	2.051	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2021.92	J/mol×K	1213.94	Joback Method
cpg	1963.25	J/mol×K	1118.51	Joback Method
cpg	1993.67	J/mol×K	1166.23	Joback Method
cpg	2073.02	J/mol×K	1309.38	Joback Method
cpg	2048.28	J/mol×K	1261.66	Joback Method
cpg	1930.41	J/mol×K	1070.80	Joback Method
cpg	1894.85	J/mol×K	1023.08	Joback Method
cpl	1206.00	J/mol×K	353.00	NIST Webbook
cps	840.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0000095	Pa×s	1023.08	Joback Method
dvisc	0.0000134	Pa×s	935.15	Joback Method
dvisc	0.0000202	Pa×s	847.21	Joback Method
dvisc	0.0004485	Pa×s	495.48	Joback Method
dvisc	0.0001455	Pa×s	583.41	Joback Method
dvisc	0.0000335	Pa×s	759.28	Joback Method
dvisc	0.0000634	Pa×s	671.35	Joback Method
hfust	88.83	kJ/mol	349.20	NIST Webbook

hfust	9.92	kJ/mol	345.40	NIST Webbook
hfust	88.83	kJ/mol	349.20	NIST Webbook
hfust	87.50	kJ/mol	225.00	NIST Webbook
hfust	87.60	kJ/mol	349.00	NIST Webbook
hfust	102.51	kJ/mol	349.20	NIST Webbook
hfust	30.54	kJ/mol	347.10	NIST Webbook
hfust	81.60	kJ/mol	350.20	NIST Webbook
hvapt	182.80	kJ/mol	298.15	Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C31 to C38 at T = 298.15 K by Correlation Gas Chromatography
hvapt	157.00 ± 2.00	kJ/mol	484.00	NIST Webbook
hvapt	124.40	kJ/mol	553.00	NIST Webbook
sfust	254.41	J/mol×K	349.20	NIST Webbook
sfust	88.01	J/mol×K	347.10	NIST Webbook
sfust	28.71	J/mol×K	345.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.30292e+02
Coeff. B	-4.15156e+04
Coeff. C	-5.72371e+01
Coeff. D	1.45802e-05
Temperature range (K), min.	535.15
Temperature range (K), max.	771.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number structures, and solvent chemistry:	https://www.doi.org/10.1016/j.fluid.2004.10.021
Observation of multiple phase transitions in some even n-alkanes by ac-Heat Capacity Solution and super-sensitive DSC:	https://www.doi.org/10.1016/j.tca.2006.06.022
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol31.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630068&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=31
Solid liquid equilibria and purity determination for binary n-alkane + naphthalene systems:	https://www.doi.org/10.1016/j.tca.2006.03.011
Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C31 to C38 at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je030236t

Legend

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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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