Hexacosane

Other names:	cerane
	n-Hexacosane
Inchi:	InChI=1S/C26H54/c1-3-5-7-9-11-13-15-17-19-21-23-25-26-24-22-20-18-16-14-12-10-8-6
InchiKey:	HMSWAIKSFDFLKN-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	366.71
CAS:	630-01-3

Physical Properties

Property code	Value	Unit	Source
gf	168.04	kJ/mol	Joback Method
hf	-579.97	kJ/mol	Joback Method
hfus	63.10	kJ/mol	Joback Method
hsub	177.00 ± 10.00	kJ/mol	NIST Webbook
hvap	139.30 ± 0.50	kJ/mol	NIST Webbook
hvap	136.40 ± 0.20	kJ/mol	NIST Webbook
hvap	131.70	kJ/mol	NIST Webbook
hvap	140.00 ± 2.20	kJ/mol	NIST Webbook
log10ws	-8.33		Aqueous Solubility Prediction Method
log10ws	-8.33		Estimated Solubility Method
logp	10.389		Crippen Method
mcvol	377.200	ml/mol	McGowan Method
pc	724.96	kPa	Joback Method
rinpol	415.90		NIST Webbook
rinpol	415.93		NIST Webbook
rinpol	415.90		NIST Webbook
ss	667.00	J/mol×K	NIST Webbook
tb	534.00 ± 5.00	K	NIST Webbook
tc	819.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	329.85	K	Aqueous Solubility Prediction Method
tt	329.26 ± 0.02	K	NIST Webbook

tt	329.18 ± 1.00	K	NIST Webbook
tt	325.70	K	Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C32)
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.12	J/mol×K	972.42	Joback Method
cpg	1240.33	J/mol×K	823.97	Joback Method
cpg	1263.20	J/mol×K	853.66	Joback Method
cpg	1284.97	J/mol×K	883.35	Joback Method
cpg	1305.68	J/mol×K	913.04	Joback Method
cpg	1325.38	J/mol×K	942.73	Joback Method
cpg	1216.30	J/mol×K	794.28	Joback Method
cpl	870.00	J/mol×K	353.00	NIST Webbook
cps	661.20	J/mol×K	298.15	NIST Webbook
cps	677.80	J/mol×K	304.00	NIST Webbook
dvisc	0.0000437	Pa×s	794.28	Joback Method
dvisc	0.0000607	Pa×s	725.70	Joback Method
dvisc	0.0000902	Pa×s	657.11	Joback Method
dvisc	0.0001471	Pa×s	588.53	Joback Method
dvisc	0.0002730	Pa×s	519.95	Joback Method
dvisc	0.0006114	Pa×s	451.36	Joback Method
dvisc	0.0018278	Pa×s	382.78	Joback Method
hfust	59.50	kJ/mol	329.50	NIST Webbook
hfust	32.20	kJ/mol	326.50	NIST Webbook
hfust	57.60	kJ/mol	328.20	NIST Webbook
hfust	59.50	kJ/mol	329.50	NIST Webbook
hfust	60.10	kJ/mol	329.10	NIST Webbook
hfust	61.10	kJ/mol	330.90	NIST Webbook
hvapt	101.60	kJ/mol	575.50	NIST Webbook

hvapt	122.00	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	131.70	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	132.00 ± 1.00	kJ/mol	414.00	NIST Webbook
hvapt	97.60	kJ/mol	475.00	NIST Webbook
hvapt	99.00 ± 3.80	kJ/mol	487.00	NIST Webbook
hvapt	94.50	kJ/mol	504.00	NIST Webbook
sfust	180.60	J/mol×K	329.50	NIST Webbook
sfust	98.70	J/mol×K	326.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.34993e+02
Coeff. B	-3.05084e+04
Coeff. C	-4.48117e+01
Coeff. D	1.43929e-05
Temperature range (K), min.	466.15
Temperature range (K), max.	685.15

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=26

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630013&Units=SI
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
Thermal conductivity of heavy even-carbon number n-alkanes (C22 to C32):	https://www.doi.org/10.1016/j.fluid.2018.08.016
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol26.mol
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/14-357-0/Hexacosane.pdf