

1-Hexadecyne

Other names:	hexadec-1-yne
Inchi:	InChI=1S/C16H30/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h1H,4-16H2,2H3
InchiKey:	UCIDYSLOTJMRAM-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	C#CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	222.41
CAS:	629-74-3

Physical Properties

Property code	Value	Unit	Source
af	0.6610		KDB
gf	306.91	kJ/mol	Joback Method
hf	-81.67	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.711		Crippen Method
mcvol	227.700	ml/mol	McGowan Method
pc	1470.00	kPa	KDB
rinpol	1664.00		NIST Webbook
tb	557.20	K	KDB
tc	724.30	K	KDB
tf	288.00 ± 2.00	K	NIST Webbook
tf	288.00	K	KDB
vc	0.893	m3/kmol	KDB
zc	0.2181010		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.39	J/mol×K	555.60	Joback Method
cpg	588.79	J/mol×K	583.37	Joback Method
cpg	606.43	J/mol×K	611.14	Joback Method
cpg	623.32	J/mol×K	638.92	Joback Method

cpg	639.50	J/mol×K	666.69	Joback Method
cpg	654.99	J/mol×K	694.46	Joback Method
cpg	669.82	J/mol×K	722.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55152e+01
Coeff. B	-5.02036e+03
Coeff. C	-9.60400e+01
Temperature range (K), min.	425.73
Temperature range (K), max.	588.05

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-1.11579e+00
Coeff. B	-7.00011e+03
Coeff. C	3.13692e+00
Coeff. D	-4.93588e-06
Temperature range (K), min.	445.15
Temperature range (K), max.	724.26

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
 Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB:	https://www.therich.org/files/research/kdb/mol/mol441.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629743&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.therich.org/research/kdb/hcprop/showprop.php?cmpid=441
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

Latest version available from:

<https://www.cheméo.com/cid/53-191-1/1-Hexadecyne.pdf>

Generated by Cheméo on 2025-12-05 15:00:51.228569966 +0000 UTC m=+4695048.758610638.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.