

Cetene

Other names:	1-CETENE 1-HEXADECENE 1-n-Hexadecene Hexadec-1-ene Hexadecene-1 Hexadecylene-1 NSC 60602 Neodene 16 n-Hexadec-1-ene «alpha»-Hexadecene Â«alphaÂ»-Hexadecene
Inchi:	InChI=1S/C16H32/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3H,1,4-16H2,2H3
InchiKey:	GQEZCXVZFLOKMC-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	C=CCCCCCCCCCCCCCC
Mol. weight [g/mol]:	224.43
CAS:	629-73-2

Physical Properties

Property code	Value	Unit	Source
af	0.7210		KDB
chl	-10540.00 ± 2.00	kJ/mol	NIST Webbook
chl	-10539.00 ± 2.00	kJ/mol	NIST Webbook
chs	-10546.00 ± 3.10	kJ/mol	NIST Webbook
gf	171.60	kJ/mol	KDB
hf	-249.30	kJ/mol	NIST Webbook
hf	-248.40 ± 2.50	kJ/mol	NIST Webbook
hf	-248.00	kJ/mol	KDB
hf	-247.20 ± 2.60	kJ/mol	NIST Webbook
hfl	-327.30 ± 2.50	kJ/mol	NIST Webbook
hfl	-330.50 ± 3.00	kJ/mol	NIST Webbook
hfl	-329.40 ± 2.10	kJ/mol	NIST Webbook
hfus	35.92	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.264		Crippen Method
mcvol	232.000	ml/mol	McGowan Method

pc	1330.00	kPa	KDB
rinpol	1591.90		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	267.80		NIST Webbook
rinpol	270.30		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1600.80		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1586.80		NIST Webbook
rinpol	1588.10		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1591.60		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1591.70		NIST Webbook
rinpol	1591.60		NIST Webbook
rinpol	1592.70		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1587.00		NIST Webbook
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rinpol	1591.90		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1594.00		NIST Webbook

rinpol	1590.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1593.20		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1588.00		NIST Webbook
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rinpol	1590.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1597.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1625.70		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1654.00		NIST Webbook
sl	587.90	J/mol×K	NIST Webbook
sl	613.88	J/mol×K	NIST Webbook
tb	547.00	K	NIST Webbook
tb	547.20	K	NIST Webbook
tb	558.00	K	KDB
tb	557.60	K	NIST Webbook
tc	717.00	K	KDB
tf	277.30	K	KDB
tt	277.51 ± 0.05	K	NIST Webbook
tt	277.45 ± 0.05	K	NIST Webbook
tt	277.30 ± 0.15	K	NIST Webbook
tt	277.39 ± 0.00	K	NIST Webbook
vc	0.912	m ³ /kmol	KDB
zc	0.2035770		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.88	J/mol×K	562.16	Joback Method
cpg	692.47	J/mol×K	723.12	Joback Method
cpg	677.27	J/mol×K	696.30	Joback Method
cpg	661.40	J/mol×K	669.47	Joback Method
cpg	644.86	J/mol×K	642.64	Joback Method
cpg	627.60	J/mol×K	615.81	Joback Method
cpg	609.62	J/mol×K	588.99	Joback Method
cpl	485.83	J/mol×K	298.15	NIST Webbook
cpl	488.88	J/mol×K	298.15	NIST Webbook
dvisc	0.0017394	Pa×s	317.29	Joback Method
dvisc	0.0008313	Pa×s	366.27	Joback Method
dvisc	0.0004729	Pa×s	415.24	Joback Method
dvisc	0.0003030	Pa×s	464.21	Joback Method
dvisc	0.0002114	Pa×s	513.19	Joback Method
dvisc	0.0047648	Pa×s	268.32	Joback Method
dvisc	0.0001570	Pa×s	562.16	Joback Method
hfust	3.87	kJ/mol	249.20	NIST Webbook
hfust	30.21	kJ/mol	277.50	NIST Webbook
hfust	30.21	kJ/mol	277.50	NIST Webbook
hfust	30.19	kJ/mol	277.51	NIST Webbook
hvapt	61.50	kJ/mol	509.50	NIST Webbook
hvapt	50.42	kJ/mol	558.00	KDB
rho	788.00	kg/m3	283.00	KDB
sfust	108.86	J/mol×K	277.50	NIST Webbook
sfust	15.53	J/mol×K	249.20	NIST Webbook
sfust	108.80	J/mol×K	277.51	NIST Webbook
srf	0.03	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60292e+01
Coeff. B	-5.35198e+03
Coeff. C	-7.81760e+01

Temperature range (K), min.	418.16
Temperature range (K), max.	577.53

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.53711e+01
Coeff. B	-1.21084e+04
Coeff. C	-1.10487e+01
Coeff. D	2.67612e-06
Temperature range (K), min.	277.51
Temperature range (K), max.	722.00

Datasets

Speed of sound, m/s

Pressure, kPa - Liquid	Temperature, K - Liquid	Speed of sound, m/s - Liquid
100.00	303.15	1314.4
100.00	313.15	1278.1
100.00	323.15	1242.5
100.00	333.15	1207.6
100.00	343.15	1173.2
100.00	353.15	1139.5
100.00	363.15	1106.4
100.00	373.15	1073.8
100.00	383.15	1041.7
100.00	393.15	1010.2
100.00	403.15	979.2
100.00	413.15	948.7
100.00	423.15	918.8
100.00	433.15	889.2
2500.00	303.15	1327.9
2500.00	313.15	1292.1
2500.00	323.15	1257.1
2500.00	333.15	1222.7
2500.00	343.15	1188.9
2500.00	353.15	1155.8

2500.00	363.15	1123.3
2500.00	373.15	1091.4
2500.00	383.15	1060.1
2500.00	393.15	1029.3
2500.00	403.15	999.1
2500.00	413.15	969.4
2500.00	423.15	940.3
2500.00	433.15	911.7
5000.00	303.15	1341.7
5000.00	313.15	1306.4
5000.00	323.15	1271.9
5000.00	333.15	1238.0
5000.00	343.15	1204.9
5000.00	353.15	1172.3
5000.00	363.15	1140.5
5000.00	373.15	1109.2
5000.00	383.15	1078.6
5000.00	393.15	1048.5
5000.00	403.15	1019.0
5000.00	413.15	990.1
5000.00	423.15	961.8
5000.00	433.15	934.0
10000.00	303.15	1368.2
10000.00	313.15	1333.9
10000.00	323.15	1300.3
10000.00	333.15	1267.5
10000.00	343.15	1235.4
10000.00	353.15	1204.0
10000.00	363.15	1173.2
10000.00	373.15	1143.1
10000.00	383.15	1113.6
10000.00	393.15	1084.8
10000.00	403.15	1056.6
10000.00	413.15	1029.0
10000.00	423.15	1002.0
10000.00	433.15	975.7
15000.00	303.15	1393.7
15000.00	313.15	1360.2
15000.00	323.15	1327.5
15000.00	333.15	1295.6
15000.00	343.15	1264.4
15000.00	353.15	1233.9
15000.00	363.15	1204.1
15000.00	373.15	1175.0

15000.00	383.15	1146.5
15000.00	393.15	1118.8
15000.00	403.15	1091.6
15000.00	413.15	1065.2
15000.00	423.15	1039.3
15000.00	433.15	1014.1
20000.00	303.15	1418.2
20000.00	313.15	1385.5
20000.00	323.15	1353.6
20000.00	333.15	1322.4
20000.00	343.15	1292.1
20000.00	353.15	1262.4
20000.00	363.15	1233.5
20000.00	373.15	1205.2
20000.00	383.15	1177.7
20000.00	393.15	1150.8
20000.00	403.15	1124.6
20000.00	413.15	1099.0
20000.00	423.15	1074.1
20000.00	433.15	1049.8
30000.00	303.15	1464.6
30000.00	313.15	1433.2
30000.00	323.15	1402.7
30000.00	333.15	1372.9
30000.00	343.15	1343.9
30000.00	353.15	1315.7
30000.00	363.15	1288.2
30000.00	373.15	1261.4
30000.00	383.15	1235.3
30000.00	393.15	1209.9
30000.00	403.15	1185.2
30000.00	413.15	1161.2
30000.00	423.15	1137.8
30000.00	433.15	1115.0
40000.00	303.15	1508.0
40000.00	313.15	1477.8
40000.00	323.15	1448.4
40000.00	333.15	1419.8
40000.00	343.15	1392.0
40000.00	353.15	1364.9
40000.00	363.15	1338.6
40000.00	373.15	1313.0
40000.00	383.15	1288.1
40000.00	393.15	1263.8

40000.00	403.15	1240.3
40000.00	413.15	1217.4
40000.00	423.15	1195.2
40000.00	433.15	1173.6
60000.00	303.15	1587.7
60000.00	313.15	1559.3
60000.00	323.15	1531.8
60000.00	333.15	1505.1
60000.00	343.15	1479.1
60000.00	353.15	1453.9
60000.00	363.15	1429.4
60000.00	373.15	1405.5
60000.00	383.15	1382.4
60000.00	393.15	1360.0
60000.00	403.15	1338.2
60000.00	413.15	1317.0
60000.00	423.15	1296.5
60000.00	433.15	1276.6
80000.00	303.15	1659.7
80000.00	313.15	1632.8
80000.00	323.15	1606.8
80000.00	333.15	1581.5
80000.00	343.15	1556.9
80000.00	353.15	1533.1
80000.00	363.15	1510.0
80000.00	373.15	1487.6
80000.00	383.15	1465.8
80000.00	393.15	1444.6
80000.00	403.15	1424.1
80000.00	413.15	1404.2
80000.00	423.15	1384.9
80000.00	433.15	1366.2
100000.00	303.15	1725.7
100000.00	313.15	1700.0
100000.00	323.15	1675.2
100000.00	333.15	1651.1
100000.00	343.15	1627.7
100000.00	353.15	1605.0
100000.00	363.15	1583.0
100000.00	373.15	1561.6
100000.00	383.15	1540.9
100000.00	393.15	1520.8
100000.00	403.15	1501.3
100000.00	413.15	1482.4

100000.00	423.15	1464.0
100000.00	433.15	1446.2
Reference		https://www.doi.org/10.1016/j.fluid.2006.01.027

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=351
The thermodynamic properties of 1-alkenes in the liquid state:	https://www.doi.org/10.1016/j.fluid.2006.01.027
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629732&Units=SI
Liquid-liquid equilibria of mixtures with ethyl lactate and various hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.02.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=351
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
KDB Pure (Korean Thermophysical Properties Databank):	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=351
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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
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
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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