1-Heptadecene

Other names:	HEXAHYDROAPLOTAXENE
	Heptadec-1-ene
	Heptadecene-
	NSC 77132
Inchi:	InChI=1S/C17H34/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3H,1,4-17H2,2H3
InchiKey:	ADOBXTDBFNCOBN-UHFFFAOYSA-N
Formula:	C17H34
SMILES:	C=CCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	238.45
CAS:	6765-39-5

Physical Properties

Property code	Value	Unit	Source
af	0.6890		KDB
gf	180.10	kJ/mol	Joback Method
hf	-268.78	kJ/mol	Joback Method
hfus	38.51	kJ/mol	Joback Method
hvap	84.90	kJ/mol	NIST Webbook
log10ws	-6.79		Crippen Method
logp	6.654		Crippen Method
mcvol	246.090	ml/mol	McGowan Method
pc	1260.00	kPa	KDB
rinpol	1689.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1692.00		NIST Webbook

rinpol	1692.00		NIST Webbook
rinpol	1693.90		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1687.60		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1686.80		NIST Webbook
rinpol	1690.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1724.60		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1726.00		NIST Webbook
tb	573.20	K	KDB
tb	573.20	K	NIST Webbook
tc	732.40	K	KDB
tf	284.00 ± 2.00	K	NIST Webbook
tf	283.85 ± 0.50	K	NIST Webbook
tf	284.00	K	KDB
tf	284.00 ± 2.00	K	NIST Webbook
vc	0.991	m3/kmol	KDB

zc	0.2049460	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.59	J/mol×K	692.15	Joback Method
cpg	749.39	J/mol×K	745.70	Joback Method
cpg	733.83	J/mol×K	718.92	Joback Method
cpg	645.34	J/mol×K	585.04	Joback Method
cpg	664.54	J/mol×K	611.82	Joback Method
cpg	682.97	J/mol×K	638.59	Joback Method
cpg	700.64	J/mol×K	665.37	Joback Method
dvisc	0.0001422	Pa×s	585.04	Joback Method
dvisc	0.0002764	Pa×s	483.22	Joback Method
dvisc	0.0001921	Pa×s	534.13	Joback Method
dvisc	0.0044659	Pa×s	279.59	Joback Method
dvisc	0.0016152	Pa×s	330.50	Joback Method
dvisc	0.0007664	Pa×s	381.41	Joback Method
dvisc	0.0004334	Pa×s	432.31	Joback Method
hvapt	72.30	kJ/mol	404.00	NIST Webbook
hvapt	55.50	kJ/mol	672.00	NIST Webbook
hvapt	51.84	kJ/mol	573.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.20	K	1.50	NIST Webbook
tbrp	433.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56682e+01

Coeff. B	-5.14021e+03
Coeff. C	-9.90300e+01
Temperature range (K), min.	433.23
Temperature range (K), max.	595.34

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.96918e+02
Coeff. B	-1.78740e+04
Coeff. C	-2.59062e+01
Coeff. D	1.03945e-05
Temperature range (K), min.	284.40
Temperature range (K), max.	736.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol352.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6765395&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=352

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

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

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
ripol:	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