

Cyclohexadecane

Inchi:	InChI=1S/C16H32/c1-2-4-6-8-10-12-14-16-15-13-11-9-7-5-3-1/h1-16H2
InchiKey:	JJWIOXUMXIOXQN-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	C1CCCCCCCCCCCCCCC1
Mol. weight [g/mol]:	224.43
CAS:	295-65-8

Physical Properties

Property code	Value	Unit	Source
chs	-10466.00 ± 1.00	kJ/mol	NIST Webbook
gf	-5.00	kJ/mol	Joback Method
hf	-360.51	kJ/mol	Joback Method
hfus	6.96	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	6.242		Crippen Method
mcvol	225.440	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	632.40	K	Joback Method
tc	887.21	K	Joback Method
tf	333.70 ± 0.30	K	NIST Webbook
tf	332.00 ± 0.50	K	NIST Webbook
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.20	J/mol×K	632.40	Joback Method
cpg	667.87	J/mol×K	674.87	Joback Method

cpg	699.07	J/mol×K	717.34	Joback Method
cpg	727.76	J/mol×K	759.80	Joback Method
cpg	753.90	J/mol×K	802.27	Joback Method
cpg	777.46	J/mol×K	844.74	Joback Method
cpg	798.39	J/mol×K	887.21	Joback Method
dvisc	0.0000081	Pa×s	632.40	Joback Method
dvisc	0.0095712	Pa×s	310.82	Joback Method
dvisc	0.0008819	Pa×s	375.13	Joback Method
dvisc	0.3604936	Pa×s	246.50	Joback Method
dvisc	0.0000465	Pa×s	503.77	Joback Method
dvisc	0.0000176	Pa×s	568.08	Joback Method
dvisc	0.0001633	Pa×s	439.45	Joback Method
hfust	4.18	kJ/mol	332.20	NIST Webbook
hfust	18.83	kJ/mol	271.20	NIST Webbook
hfust	1.26	kJ/mol	283.20	NIST Webbook
hfust	4.18	kJ/mol	332.20	NIST Webbook
sfust	69.42	J/mol×K	271.20	NIST Webbook
sfust	4.43	J/mol×K	283.20	NIST Webbook
sfust	12.59	J/mol×K	332.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	0.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36568e+01
Coeff. B	-4.36416e+03
Coeff. C	-9.11500e+01
Temperature range (K), min.	417.59
Temperature range (K), max.	614.10

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C295658&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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