

Cyclooctadecane

Inchi:	InChI=1S/C18H36/c1-2-4-6-8-10-12-14-16-18-17-15-13-11-9-7-5-3-1/h1-18H2
InchiKey:	JNFIMRWCDIOUMT-UHFFFAOYSA-N
Formula:	C18H36
SMILES:	C1CCCCCCCCCCCCCCCCC1
Mol. weight [g/mol]:	252.48
CAS:	296-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-12.36	kJ/mol	Joback Method
hf	-414.11	kJ/mol	Joback Method
hfus	7.94	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	7.022		Crippen Method
mcvol	253.620	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
tb	686.70	K	Joback Method
tc	946.78	K	Joback Method
tf	346.00 ± 3.00	K	NIST Webbook
tf	346.00 ± 2.00	K	NIST Webbook
tf	345.00 ± 3.00	K	NIST Webbook
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.84	J/mol×K	686.70	Joback Method
cpg	798.02	J/mol×K	730.05	Joback Method
cpg	830.21	J/mol×K	773.39	Joback Method
cpg	859.37	J/mol×K	816.74	Joback Method
cpg	885.43	J/mol×K	860.09	Joback Method
cpg	908.34	J/mol×K	903.43	Joback Method
cpg	928.03	J/mol×K	946.78	Joback Method

dvisc	0.0055331	Pa×s	332.78	Joback Method
dvisc	0.3047131	Pa×s	262.00	Joback Method
dvisc	0.0004100	Pa×s	403.57	Joback Method
dvisc	0.0000660	Pa×s	474.35	Joback Method
dvisc	0.0000171	Pa×s	545.13	Joback Method
dvisc	0.0000060	Pa×s	615.92	Joback Method
dvisc	0.0000026	Pa×s	686.70	Joback Method
hfust	9.87	kJ/mol	346.00	NIST Webbook
hfust	9.87	kJ/mol	346.20	NIST Webbook
sfust	28.40	J/mol×K	346.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32047e+01
Coeff. B	-4.36112e+03
Coeff. C	-9.59000e+01
Temperature range (K), min.	433.52
Temperature range (K), max.	648.41

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C296184&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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