1-Octadecyne

Other names: octadecyne
Inchi: InChI=1S/C18H34/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h1H,4-18H2,2H3
InchiKey: IYDNQWWOZQLMRH-UHFFFAOYSA-N
Formula: C18H34
SMILES: C#CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 250.46
CAS: 629-89-0

Physical Properties

Property code	Value	Unit	Source
af	0.7150		KDB
gf	323.75	kJ/mol	Joback Method
hf	-122.95	kJ/mol	Joback Method
hfus	45.35	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.491		Crippen Method
mcvol	255.880	ml/mol	McGowan Method
pc	1280.00	kPa	KDB
rinpol	1238.00		NIST Webbook
tb	586.00	K	NIST Webbook
tb	586.20	K	KDB
tc	747.30	K	KDB
tf	300.00	K	KDB
vc	1.006	m3/kmol	KDB
zc	0.2071380		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.32	J/mol×K	739.15	Joback Method
cpg	678.57	J/mol×K	601.36	Joback Method
cpg	697.89	J/mol×K	628.92	Joback Method
cpg	716.39	J/mol×K	656.48	Joback Method

cpg	734.12	J/mol×K	684.04	Joback Method
cpg	751.08	J/mol×K	711.60	Joback Method
cpg	782.86	J/mol×K	766.71	Joback Method
hvapt	64.90	kJ/mol	536.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54537e+01
Coeff. B	-5.22966e+03
Coeff. C	-1.04102e+02
Temperature range (K), min.	448.93
Temperature range (K), max.	619.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.77078e-01
Coeff. B	-7.38386e+03
Coeff. C	2.96884e+00
Coeff. D	-4.11555e-06
Temperature range (K), min.	469.15
Temperature range (K), max.	747.33

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol443.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629890&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=443
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
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
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