1-Heptadecyne

Inchi: InChI=1S/C17H32/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h1H,4-17H2,2H3
InchiKey: DQDNKQWGBZFFRA-UHFFFAOYSA-N
Formula: C17H32
SMILES: C#CCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 236.44
CAS: 26186-00-5

Physical Properties

Property code	Value	Unit	Source
af	0.6900		KDB
gf	315.33	kJ/mol	Joback Method
hf	-102.31	kJ/mol	Joback Method
hfus	42.76	kJ/mol	Joback Method
hvap	53.29	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.101		Crippen Method
mcvol	241.790	ml/mol	McGowan Method
pc	1370.00	kPa	KDB
tb	572.20	K	KDB
tc	736.20	K	KDB
tf	295.00	K	KDB
vc	0.950	m3/kmol	KDB
zc	0.2125120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.76	J/mol×K	578.48	Joback Method
cpg	642.63	J/mol×K	606.12	Joback Method
cpg	660.73	J/mol×K	633.77	Joback Method
cpg	678.05	J/mol×K	661.41	Joback Method
cpg	694.65	J/mol×K	689.06	Joback Method
cpg	710.53	J/mol×K	716.70	Joback Method
cpg	725.73	J/mol×K	744.35	Joback Method

hvapt	62.70	kJ/mol	522.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54993e+01
Coeff. B	-5.13420e+03
Coeff. C	-1.00210e+02
Temperature range (K), min.	437.73
Temperature range (K), max.	604.17

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.20978e-01
Coeff. B	-7.30684e+03
Coeff. C	2.92546e+00
Coeff. D	-4.59123e-06
Temperature range (K), min.	457.15
Temperature range (K), max.	736.21

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol442.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26186005&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=442
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility