1-Pentadecyne

Other names:	1-Penatdecyne
	pentadec-1-yne
Inchi:	InChI=1S/C15H28/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h1H,4-15H2,2H3
InchiKey:	DONJGKADZJEXRJ-UHFFFAOYSA-N
Formula:	C15H28
SMILES:	C#CCCCCCCCCCCCCC
Mol. weight [g/mol]:	208.38
CAS:	765-13-9

Physical Properties

Property code	Value	Unit	Source
af	0.6280		KDB
gf	298.49	kJ/mol	Joback Method
hf	-61.03	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.321		Crippen Method
mcvol	213.610	ml/mol	McGowan Method
pc	1590.00	kPa	KDB
rinpol	1526.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	541.20	K	KDB
tc	711.40	K	KDB
tf	283.00	K	KDB
vc	0.838	m3/kmol	KDB
zc	0.2251290		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.58	J/mol×K	532.72	Joback Method
cpg	536.45	J/mol×K	560.65	Joback Method

cpg	553.58	J/mol×K	588.59	Joback Method
cpg	569.98	J/mol×K	616.52	Joback Method
cpg	585.70	J/mol×K	644.45	Joback Method
cpg	600.74	J/mol×K	672.38	Joback Method
cpg	615.14	J/mol×K	700.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55051e+01
Coeff. B	-4.88992e+03
Coeff. C	-9.15920e+01
Temperature range (K), min.	412.93
Temperature range (K), max.	571.30

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.16522e+02
Coeff. B	-1.23534e+04
Coeff. C	-1.44225e+01
Coeff. D	5.78566e-06
Temperature range (K), min.	413.15
Temperature range (K), max.	711.41

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765139&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=440
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol440.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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