n-Pentadecanol

Other names:	1-Pentadecanol
	N-PENTADECYL ALCOHOL
	Neodol 5
	PENTADECANOL
	PENTADECYL ALCOHOL
	Pentadecan-1-ol
	n-1-Pentadecanol
Inchi:	InChI=1S/C15H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h16H,2-15H2,1H3
InchiKey:	REIUXOLGHVXAEO-UHFFFAOYSA-N
Formula:	C15H32O
SMILES:	CCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	228.41
CAS:	629-76-5

Physical Properties

Property code	Value	Unit	Source
af	1.0150		KDB
chs	-9817.70	kJ/mol	NIST Webbook
gf	-61.40	kJ/mol	Joback Method
hf	-505.16	kJ/mol	Joback Method
hfs	-658.30 ± 0.60	kJ/mol	NIST Webbook
hfus	103.50	kJ/mol	Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography

hfus	21.40	kJ/mol	Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlationos for the heat capacity and the entropy of liquid n-alcohols
hvap	102.50	kJ/mol	NIST Webbook
hvap	103.50 ± 3.30	kJ/mol	NIST Webbook
hvap	107.20	kJ/mol	NIST Webbook
log10ws	-6.35		Aqueous Solubility Prediction Method
log10ws	-6.35		Estimated Solubility Method
logp	5.070		Crippen Method
mcvol	228.080	ml/mol	McGowan Method
pc	1520.00	kPa	KDB
rinpol	1765.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	296.98		NIST Webbook
rinpol	298.56		NIST Webbook
rinpol	1765.10		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1765.10		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1787.00		NIST Webbook

rinpol	1791.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1788.90		NIST Webbook
rinpol	1755.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2243.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2272.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2254.00		NIST Webbook
tb	578.00	K	KDB
tc	722.50	K	KDB
tf	316.92 ± 0.05	K	NIST Webbook
tf	317.00	K	KDB
tf	317.65 ± 0.40	K	NIST Webbook
tf	311.70 ± 2.00	K	NIST Webbook
tf	316.61 ± 0.05	K	NIST Webbook
tf	318.98	K	Aqueous Solubility Prediction Method
vc	0.894	m3/kmol	KDB
zc	0.2263340		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.95	J/mol×K	634.78	Joback Method
cpg	653.34	J/mol×K	661.23	Joback Method
cpg	669.08	J/mol×K	687.68	Joback Method
cpg	684.18	J/mol×K	714.14	Joback Method
cpg	698.65	J/mol×K	740.59	Joback Method
cpg	712.53	J/mol×K	767.04	Joback Method
cpg	725.83	J/mol×K	793.49	Joback Method
cpl	567.40	J/mol×K	323.15	NIST Webbook
cps	537.30	J/mol×K	358.00	NIST Webbook
cps	400.00	J/mol×K	298.15	NIST Webbook
cps	535.00	J/mol×K	318.00	NIST Webbook
dvisc	0.0000810	Pa×s	582.25	Joback Method
dvisc	0.0001456	Pa×s	529.73	Joback Method
dvisc	0.0002978	Pa×s	477.20	Joback Method
dvisc	0.0000497	Pa×s	634.78	Joback Method
dvisc	0.0007268	Pa×s	424.68	Joback Method
dvisc	0.0104331	Pa×s	319.63	Joback Method
dvisc	0.0022817	Pa×s	372.15	Joback Method
hfust	54.73	kJ/mol	316.60	NIST Webbook
hfust	54.73	kJ/mol	316.60	NIST Webbook
hfust	53.62	kJ/mol	316.90	NIST Webbook
hfust	29.60	kJ/mol	316.40	NIST Webbook
hfust	23.64	kJ/mol	316.00	NIST Webbook
hvapt	95.50	kJ/mol	338.50	NIST Webbook
hvapt	92.40	kJ/mol	368.00	NIST Webbook
hvapt	75.00	kJ/mol	519.00	NIST Webbook
hvapt	72.40	kJ/mol	518.50	NIST Webbook
sfust	74.81	J/mol×K	316.00	NIST Webbook
sfust	172.86	J/mol×K	316.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72985e+01

Coeff. B	-5.96038e+03
Coeff. C	-1.03335e+02
Temperature range (K), min.	453.72
Temperature range (K), max.	600.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.55623e+02
Coeff. B	-2.20313e+04
Coeff. C	-3.41892e+01
Coeff. D	1.32387e-05
Temperature range (K), min.	438.15
Temperature range (K), max.	600.15

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlations for the heat capacity and enthalpy of liquid n-alcohols:	https://www.doi.org/10.1021/je0255240
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629765&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=855
KDB:	https://www.cheric.org/files/research/kdb/mol/mol855.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility