n-Tridecan-1-ol

Other names:	1-HYDROXYTRIDECANE
	1-Tridecanol
	N-TRIDECYL ALCOHOL
	TRIDECANOL
	Tridecan-1-ol
	Tridecyl alcohol
	n-Tridecanol
Inchi:	InChI=1S/C13H28O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h14H,2-13H2,1H3
InchiKey:	XFRVVPUIAFSTFO-UHFFFAOYSA-N
Formula:	C13H28O
SMILES:	CCCCCCCCCCCCCO
Mol. weight [g/mol]:	200.36
CAS:	112-70-9

Physical Properties

Property code	Value	Unit	Source
af	0.9890		KDB
chs	-8517.80 ± 0.90	kJ/mol	NIST Webbook
gf	-78.24	kJ/mol	Joback Method
hf	-463.88	kJ/mol	Joback Method
hfs	-599.50 ± 0.90	kJ/mol	NIST Webbook
hfus	94.70	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	1.50	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	95.80	kJ/mol	NIST Webbook
hvap	94.70 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.53		Crippen Method
logp	4.290		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1935.00	kPa	KDB
rinpol	1593.00		NIST Webbook
rinpol	266.83		NIST Webbook
rinpol	268.36		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	220.20		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	266.83		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1585.50		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1563.60		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1572.00		NIST Webbook

rinpol	1585.30		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1599.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2077.00		NIST Webbook
tb	547.20	K	KDB
tc	734.00	K	KDB
tf	305.60	K	KDB
tf	301.70 ± 1.00	K	NIST Webbook
tf	304.89 ± 0.05	K	NIST Webbook
tf	304.63 ± 0.04	K	NIST Webbook
tf	303.50 ± 0.05	K	NIST Webbook
tf	303.05 ± 0.50	K	NIST Webbook
vc	0.782	m3/kmol	KDB
zc	0.2481030		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.21	J/mol×K	720.48	Joback Method
cpg	573.73	J/mol×K	667.90	Joback Method
cpg	559.66	J/mol×K	641.61	Joback Method
cpg	545.01	J/mol×K	615.31	Joback Method
cpg	529.76	J/mol×K	589.02	Joback Method
cpg	612.65	J/mol×K	746.78	Joback Method
cpg	587.24	J/mol×K	694.19	Joback Method
cpl	476.00	J/mol×K	305.00	NIST Webbook

cpl	487.50	J/mol×K	313.15	NIST Webbook
cps	378.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0002143	Pa×s	491.71	Joback Method
dvisc	0.0010971	Pa×s	394.40	Joback Method
dvisc	0.0035036	Pa×s	345.75	Joback Method
dvisc	0.0163656	Pa×s	297.09	Joback Method
dvisc	0.0004434	Pa×s	443.06	Joback Method
dvisc	0.0000718	Pa×s	589.02	Joback Method
dvisc	0.0001181	Pa×s	540.37	Joback Method
hfust	18.74	kJ/mol	306.60	NIST Webbook
hfust	44.78	kJ/mol	304.70	NIST Webbook
hvapt	91.10	kJ/mol	327.50	NIST Webbook
hvapt	87.40	kJ/mol	343.00	NIST Webbook
hvapt	69.20	kJ/mol	499.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76371e+01
Coeff. B	-5.80912e+03
Coeff. C	-9.50510e+01
Temperature range (K), min.	429.88
Temperature range (K), max.	566.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.67240e+02
Coeff. B	-2.16241e+04
Coeff. C	-3.61080e+01

Coeff. D	1.49630e-05
Temperature range (K), min.	303.75
Temperature range (K), max.	731.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol853.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-Heneicosanol, 1-Docosanol, 1-Tetracosanol, and 1-Hexacosanol at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112709&Units=SI
Heat capacities and derived thermodynamic functions of 1-pentadecanol and 1-heptadecanol between 10 K and 370 K and heat capacities of cholesterol at T = 298.15 K by adiabatic calorimetry:	https://www.doi.org/10.1021/je025524o
Kdb Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=853
Correlation Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlationos for the heat capacity and the entropy of liquid n-alcohols:	

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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure

rinpol:	Non-polar retention indices
ripol:	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