

Tridecane

Other names:	Tridecane, n- n-Tridecane
Inchi:	InChI=1S/C13H28/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey:	IIYFAKIEWZDVMP-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCCCCCCCCCC
Mol. weight [g/mol]:	184.36
CAS:	629-50-5

Physical Properties

Property code	Value	Unit	Source
af	0.6190		KDB
chl	-8739.70 ± 1.40	kJ/mol	NIST Webbook
gf	58.49	kJ/mol	KDB
hf	-311.70	kJ/mol	KDB
hf	-311.50 ± 1.60	kJ/mol	NIST Webbook
hfl	-377.70 ± 1.60	kJ/mol	NIST Webbook
hfus	29.43	kJ/mol	Joback Method
hsub	91.40	kJ/mol	NIST Webbook
hvap	66.40 ± 0.30	kJ/mol	NIST Webbook
hvap	66.50 ± 0.20	kJ/mol	NIST Webbook
hvap	66.43	kJ/mol	NIST Webbook
hvap	66.70	kJ/mol	NIST Webbook
hvap	66.20	kJ/mol	NIST Webbook
log10ws	-5.26		Crippen Method
logp	5.317		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1700.00 ± 100.00	kPa	NIST Webbook
pc	1679.00 ± 20.00	kPa	NIST Webbook
pc	1680.00	kPa	KDB
pc	1725.00 ± 34.47	kPa	NIST Webbook
pc	1720.00	kPa	NIST Webbook
rhoc	221.23 ± 18.44	kg/m3	NIST Webbook
rhoc	224.92 ± 5.53	kg/m3	NIST Webbook
rinpol	221.55		NIST Webbook
rinpol	218.83		NIST Webbook
sg	661.45	J/mol×K	NIST Webbook

sl	522.87	J/mol×K	NIST Webbook
tb	507.75 ± 0.40	K	NIST Webbook
tb	506.00 ± 2.00	K	NIST Webbook
tb	507.00 ± 1.50	K	NIST Webbook
tb	505.00 ± 4.00	K	NIST Webbook
tb	508.62	K	KDB
tb	507.20	K	NIST Webbook
tb	508.60	K	NIST Webbook
tb	507.15 ± 0.60	K	NIST Webbook
tb	508.60 ± 0.30	K	NIST Webbook
tb	507.00 ± 4.00	K	NIST Webbook
tc	675.80 ± 0.40	K	NIST Webbook
tc	674.90 ± 1.00	K	NIST Webbook
tc	676.20 ± 0.60	K	NIST Webbook
tc	676.20 ± 1.00	K	NIST Webbook
tc	675.80	K	NIST Webbook
tc	674.00 ± 0.80	K	NIST Webbook
tc	675.98	K	NIST Webbook
tc	675.80 ± 0.40	K	NIST Webbook
tc	675.00	K	KDB
tc	675.00 ± 1.00	K	NIST Webbook
tc	676.00 ± 0.60	K	NIST Webbook
tf	267.76 ± 0.02	K	NIST Webbook
tf	266.00 ± 2.00	K	NIST Webbook
tf	267.74 ± 0.02	K	NIST Webbook
tf	267.74 ± 0.02	K	NIST Webbook
tf	267.76 ± 0.01	K	NIST Webbook
tf	267.00 ± 2.00	K	NIST Webbook
tf	267.73 ± 0.10	K	NIST Webbook
tf	267.76 ± 0.10	K	NIST Webbook
tf	267.82 ± 0.07	K	NIST Webbook
tf	267.80 ± 0.20	K	NIST Webbook
tf	267.74 ± 0.08	K	NIST Webbook
tf	269.01	K	Influence of High Pressure on the Liquidus Curve Shape in Binary Hydrocarbon Mixtures: Experimental Data, Correlation, and Prediction
tf	267.76	K	KDB
tf	267.90 ± 0.50	K	NIST Webbook
tf	267.90 ± 0.60	K	NIST Webbook
tf	267.70 ± 1.00	K	NIST Webbook
tf	265.00 ± 3.00	K	NIST Webbook
tf	267.00 ± 3.00	K	NIST Webbook
tf	266.00 ± 3.00	K	NIST Webbook

tf	267.00 ± 2.00	K	NIST Webbook
tf	269.01	K	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
tf	267.85 ± 0.50	K	NIST Webbook
tf	267.74 ± 0.08	K	NIST Webbook
tt	267.79 ± 0.02	K	NIST Webbook
tt	267.78 ± 0.20	K	NIST Webbook
tt	267.79 ± 0.40	K	NIST Webbook
tt	267.79 ± 0.20	K	NIST Webbook
tt	267.78 ± 0.40	K	NIST Webbook
tt	267.78 ± 0.05	K	NIST Webbook
vc	0.823	m3/kmol	NIST Webbook
vc	0.823	m3/kmol	KDB
zc	0.2463590		KDB
zra	0.25		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.94	J/mol×K	523.55	Joback Method
cpg	550.76	J/mol×K	657.11	Joback Method
cpg	536.40	J/mol×K	630.40	Joback Method
cpg	521.46	J/mol×K	603.69	Joback Method
cpg	505.91	J/mol×K	576.98	Joback Method
cpg	489.74	J/mol×K	550.26	Joback Method
cpg	455.48	J/mol×K	496.84	Joback Method
cpl	409.40	J/mol×K	303.15	NIST Webbook
cpl	406.89	J/mol×K	298.15	NIST Webbook
dvisc	0.0003823	Pa×s	409.98	Joback Method
dvisc	0.0010457	Pa×s	323.13	Joback Method
dvisc	0.0005957	Pa×s	366.55	Joback Method
dvisc	0.0001987	Pa×s	496.84	Joback Method
dvisc	0.0002672	Pa×s	453.41	Joback Method
dvisc	0.0021859	Pa×s	279.70	Joback Method
dvisc	0.0059922	Pa×s	236.27	Joback Method
hfust	28.49	kJ/mol	267.80	NIST Webbook
hfust	7.66	kJ/mol	255.00	NIST Webbook
hfust	28.49	kJ/mol	267.80	NIST Webbook

hfust	28.90	kJ/mol	267.70	NIST Webbook
hvapt	64.90	kJ/mol	314.00	NIST Webbook
hvapt	63.30	kJ/mol	334.00	NIST Webbook
hvapt	64.20	kJ/mol	324.00	NIST Webbook
hvapt	62.40	kJ/mol	344.00	NIST Webbook
hvapt	65.30	kJ/mol	309.00	NIST Webbook
hvapt	45.65	kJ/mol	507.80	KDB
hvapt	62.30	kJ/mol	349.00	NIST Webbook
hvapt	54.50	kJ/mol	464.00	NIST Webbook
hvapt	65.60	kJ/mol	308.00	NIST Webbook
hvapt	64.60	kJ/mol	318.00	NIST Webbook
hvapt	61.70	kJ/mol	348.00	NIST Webbook
rfi	1.41550		318.15	Thermodynamic properties of (an ester + an alkane). XVI. Experimental HEm and V Em values and a new correlation method for (an alkyl ethanoate + an n-alkane) at 318.15 K
rhoI	720.20	kg/m3	344.15	High-pressure densities and interfacial tensions of binary systems containing carbon dioxide + n-alkanes: (n-Dodecane, n-tridecane, n-tetradecane)
rhoI	756.00	kg/m3	293.00	KDB
sfust	106.27	J/mol×K	267.80	NIST Webbook
sfust	30.04	J/mol×K	255.00	NIST Webbook
srf	0.02	N/m	293.15	Density, Refractive Index, Viscosity, and Surface Tension of Binary Mixtures of exo-Tetrahydrodicyclopentadiene with Some n-Alkanes from (293.15 to 313.15) K
srf	0.03	N/m	293.20	KDB

srf	0.02	N/m	303.15	Density, Refractive Index, Viscosity, and Surface Tension of Binary Mixtures of exo-Tetrahydrodicyclopentadiene with Some n-Alkanes from (293.15 to 313.15) K
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	268.21	K	100.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction
tfp	293.15	K	133010.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction
tfp	303.15	K	197120.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction
tfp	313.15	K	265400.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction

tfp	323.15	K	337830.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction
tfp	333.15	K	414420.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction
tfp	343.15	K	495170.00	High pressure (solid + liquid) equilibria of n-alkane mixtures: experimental results, correlation and prediction

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48906e+01
Coeff. B	-4.50848e+03
Coeff. C	-6.97210e+01
Temperature range (K), min.	378.46
Temperature range (K), max.	540.38

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.01620e+02
Coeff. B	-1.09918e+04
Coeff. C	-1.23037e+01
Coeff. D	4.95821e-06
Temperature range (K), min.	267.76
Temperature range (K), max.	675.80

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
313.01	1023.00	743.49
313.01	2030.00	744.27
313.01	3025.00	745.05
313.01	4027.00	745.74
313.01	5014.00	746.51
313.01	6024.00	747.18
313.01	7021.00	747.95
313.01	8036.00	748.69
313.01	9019.00	749.41
313.01	10018.00	750.14
313.01	11030.00	750.86
313.01	12006.00	751.51
313.01	13017.00	752.24
313.01	14035.00	752.95
313.01	15021.00	753.59
313.01	16019.00	754.27
313.01	17019.00	754.94
313.01	18024.00	755.61
313.01	19025.00	756.27
313.01	20043.00	756.91
313.01	21011.00	757.52
313.01	22020.00	758.16
313.01	23018.00	758.79
313.01	24004.00	759.44
313.01	25036.00	760.12
322.92	1017.00	736.15
322.92	2006.00	736.94
322.92	3025.00	737.83
322.92	4021.00	738.62
322.92	5021.00	739.42
322.92	6043.00	740.18
322.92	7018.00	740.9
322.92	8022.00	741.72

322.92	9008.00	742.44
322.92	10012.00	743.18
322.92	11015.00	743.93
322.92	12006.00	744.71
322.92	13030.00	745.38
322.92	14010.00	746.12
322.92	15026.00	746.81
322.92	16024.00	747.53
322.92	17016.00	748.22
322.92	18010.00	748.89
322.92	19007.00	749.56
322.92	20023.00	750.22
322.92	21020.00	750.92
322.92	22010.00	751.57
322.92	23040.00	752.26
322.92	24006.00	752.95
322.92	25006.00	753.6
332.78	1015.00	729.19
332.78	2020.00	730.06
332.78	3022.00	730.83
332.78	4016.00	731.63
332.78	5020.00	732.47
332.78	6016.00	733.27
332.78	7006.00	734.09
332.78	8018.00	734.9
332.78	9013.00	735.71
332.78	10008.00	736.52
332.78	11016.00	737.3
332.78	12007.00	738.05
332.78	13012.00	738.79
332.78	14021.00	739.55
332.78	15011.00	740.26
332.78	16020.00	741.03
332.78	17015.00	741.74
332.78	18005.00	742.47
332.78	19017.00	743.19
332.78	20014.00	743.89
332.78	21016.00	744.66
332.78	22046.00	745.35
332.78	22994.00	745.97
332.78	24032.00	746.67
332.78	25030.00	747.38
342.64	1022.00	722.03
342.64	2014.00	722.93

342.64	3025.00	723.84
342.64	4021.00	724.7
342.64	5020.00	725.59
342.64	6020.00	726.44
342.64	7008.00	727.27
342.64	8026.00	728.15
342.64	9007.00	728.98
342.64	10010.00	729.81
342.64	11012.00	730.63
342.64	12014.00	731.46
342.64	13011.00	732.27
342.64	14008.00	733.03
342.64	15029.00	733.84
342.64	16006.00	734.58
342.64	17016.00	735.35
342.64	18019.00	736.09
342.64	19006.00	736.85
342.64	20001.00	737.59
342.64	21023.00	738.34
342.64	22008.00	739.06
342.64	23005.00	739.79
342.64	24032.00	740.52
342.64	25024.00	741.14
352.47	1013.00	714.88
352.47	2022.00	715.88
352.47	3010.00	716.8
352.47	4020.00	717.71
352.47	5019.00	718.65
352.47	6011.00	719.55
352.47	7017.00	720.47
352.47	8014.00	721.35
352.47	9022.00	722.24
352.47	10031.00	723.11
352.47	11010.00	723.98
352.47	12003.00	724.82
352.47	13024.00	725.71
352.47	14013.00	726.54
352.47	15007.00	727.34
352.47	16016.00	728.16
352.47	17007.00	728.94
352.47	18020.00	729.77
352.47	19011.00	730.53
352.47	20013.00	731.29
352.47	21032.00	732.07

352.47	22020.00	732.84
352.47	23020.00	733.6
352.47	24021.00	734.36
352.47	25024.00	735.14
362.25	1020.00	707.72
362.25	2026.00	708.74
362.25	3018.00	709.77
362.25	4006.00	710.71
362.25	5021.00	711.73
362.25	6019.00	712.7
362.25	7029.00	713.67
362.25	8017.00	714.54
362.25	9011.00	715.51
362.25	10011.00	716.42
362.25	11021.00	717.35
362.25	12018.00	718.24
362.25	13014.00	719.11
362.25	14000.00	719.97
362.25	15017.00	720.85
362.25	16026.00	721.7
362.25	17019.00	722.52
362.25	18034.00	723.36
362.25	19016.00	724.17
362.25	20004.00	725.0
362.25	21015.00	725.8
362.25	22022.00	726.63
362.25	23008.00	727.42
362.25	24034.00	728.22
362.25	25010.00	729.02

Reference

<https://www.doi.org/10.1016/j.fluid.2007.04.023>

Pressure, kPa	Temperature, K	Mass density, kg/m3
100.00	283.15	763.6
100.00	288.15	760.0
100.00	293.15	756.4
100.00	298.15	752.6
100.00	303.15	749.2
100.00	308.15	745.6
100.00	313.15	742.0
100.00	318.15	738.4
100.00	323.15	734.8
10000.00	283.15	769.7

10000.00	288.15	766.2
10000.00	293.15	762.8
10000.00	298.15	759.3
10000.00	303.15	755.9
10000.00	308.15	752.5
10000.00	313.15	749.1
10000.00	318.15	745.7
10000.00	323.15	742.3
20000.00	283.15	775.5
20000.00	288.15	772.1
20000.00	293.15	768.9
20000.00	298.15	765.5
20000.00	303.15	762.3
20000.00	308.15	759.1
20000.00	313.15	755.7
20000.00	318.15	752.5
20000.00	323.15	749.3
30000.00	283.15	781.0
30000.00	288.15	777.7
30000.00	293.15	774.6
30000.00	298.15	771.4
30000.00	303.15	768.3
30000.00	308.15	765.1
30000.00	313.15	761.9
30000.00	318.15	758.8
30000.00	323.15	755.7
40000.00	283.15	786.1
40000.00	288.15	783.0
40000.00	293.15	780.0
40000.00	298.15	776.8
40000.00	303.15	773.8
40000.00	308.15	770.8
40000.00	313.15	767.7
40000.00	318.15	764.7
40000.00	323.15	761.8
50000.00	283.15	791.0
50000.00	288.15	788.0
50000.00	293.15	785.1
50000.00	298.15	782.0
50000.00	303.15	779.0
50000.00	308.15	776.1
50000.00	313.15	773.2
50000.00	318.15	770.3
50000.00	323.15	767.3

60000.00	283.15	795.6
60000.00	288.15	792.7
60000.00	293.15	789.8
60000.00	298.15	786.9
60000.00	303.15	784.0
60000.00	308.15	781.1
60000.00	313.15	778.3
60000.00	318.15	775.4
60000.00	323.15	772.6

Reference

<https://www.doi.org/10.1021/je8006875>

Sources

Infinite dilution activity coefficients, specific retention volumes and liquid-liquid equilibria of the Ternary Systems Consisting of 2,2,4,4-Tetrahydrothiophene 1,1-Dioxide and High Pressure Densities and Interfacial Tensions of Binary Systems Containing Carbon Dioxide and Alkanes Equilibria in CO₂-alkane mixtures and evaluation of the Poynting and Poynting-Frication Ionic Liquids for Separation Problems.

Oxygenated ionic liquids using gas chromatography: Measurement and Correlation of High Pressure Phase Equilibria for CO₂ + Alkanes and CO₂ + esters of carboxylic acids (an alkane). XVI. Experimental HEM and VLE Data for CO₂ + n-Alkane at 318.15 K:

(p, rho, T) Behavior for the Binary Mixtures Carbon Dioxide + Heptane and Influence of High Pressure on the Liquidus Curve Shape in Binary Hydrocarbon and the effect of mutual interaction between and prediction: Density, Refractive Index, Viscosity, and Surface Tension of Binary Mixtures Based on Carbon Dioxide + Cyclohexane with Some n-Alkane and Azobenzene and Tetrahydrofuran Based on Cyclohexane mixtures: experimental measurement and correlation of the interfacial tension for paraffin + CO₂ and (CO₂ + n) and gas-liquid equilibrium liquid-liquid equilibria binary acetonitrile + n-alkane systems:

Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and VLE Data for CO₂ + Propanoate Cyclic Ether and Cationic Liquids Solution Phase Diagrams near a liquid-liquid critical point I. First-order phase diagrams of binary systems containing n-alkanes, or cyclohexane, and 2,3-pentanedione at atmospheric and high pressure: Interfacial Tension Measurement and Calculation of (Carbon Dioxide + n-Alkane) Binary Mixtures:

<https://www.doi.org/10.1016/j.fluid.2006.07.015>

<https://www.doi.org/10.1021/je200465z>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=13>

<https://www.doi.org/10.1016/j.fluid.2014.07.039>

<https://www.doi.org/10.1016/j.fluid.2007.04.023>

<https://www.doi.org/10.1021/je201129y>

<https://www.doi.org/10.1016/j.fluid.2014.11.020>

https://www.chemedoc.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1021/acs.jced.7b00517>

<https://www.doi.org/10.1016/j.jct.2003.11.008>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1021/je400056z>

<https://www.doi.org/10.1021/je050039p>

<https://www.doi.org/10.1016/j.fluid.2014.06.021>

<https://www.doi.org/10.1021/je200757a>

<https://www.doi.org/10.1021/je9003178>

<https://www.doi.org/10.1016/j.fluid.2004.11.020>

<https://www.doi.org/10.1016/j.fluid.2017.02.012>

<https://www.doi.org/10.1016/j.fluid.2010.10.013>

<https://www.thermo.com/files/research/kdb/mol/mol13.mol>

<https://www.doi.org/10.1016/j.jct.2004.12.014>

<https://www.doi.org/10.1021/je900838a>

<https://www.doi.org/10.1016/j.fluid.2007.05.017>

<https://www.doi.org/10.1016/j.fluid.2006.02.001>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1021/acs.jced.7b00159>

CO₂ and alkane minimum miscible pressure estimation by the NIST-Webbook extrapolation of interfacial tension:

<https://www.doi.org/10.1016/j.fluid.2019.05.002>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C629505&Units=SI>

Activity coefficients at infinite dilution of organic solutes in tripropylphosphate based ionic liquids using gas-liquid chromatography and solvent heat capacity measurement of Organic Compounds in Four New Ionic-Liquid Based Ionic Liquids:

<https://www.doi.org/10.1016/j.jct.2015.02.023>

<https://www.doi.org/10.1021/je8006875>

<https://www.doi.org/10.1021/je200195q>

https://en.wikipedia.org/wiki/Joback_method

<https://www.doi.org/10.1016/j.jct.2017.08.031>

Experiment and correlation of the equilibrium interfacial tension for paraffin + CO₂ modified with ethanol:

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rfi:	Refractive Index
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature

vc: Critical Volume
zc: Critical Compressibility
zra: Rackett Parameter

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