4-Heptanol

Other names:	CH3(CH2)2CHOH(CH2)2CH3
	Dipropylcarbinol
	Heptanol-4
	di-n-Propylcarbinol
	heptan-4-ol
	n-Heptan-4-ol
Inchi:	InChI=1S/C7H16O/c1-3-5-7(8)6-4-2/h7-8H,3-6H2,1-2H3
InchiKey:	YVBCULSIZWMTFY-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(O)CCC
Mol. weight [g/mol]:	116.20
CAS:	589-55-9

Physical Properties

Property code	Value	Unit	Source
cpl	306.77	J/mol×K	Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols
gf	-131.20	kJ/mol	Joback Method
hf	-354.80 ± 2.10	kJ/mol	NIST Webbook
hfl	-416.30 ± 0.67	kJ/mol	NIST Webbook
hfus	14.45	kJ/mol	Joback Method
hvap	62.40 ± 0.30	kJ/mol	NIST Webbook
ie	10.03	eV	NIST Webbook
ie	9.61 ± 0.03	eV	NIST Webbook
log10ws	-1.40		Estimated Solubility Method
log10ws	-1.40		Aqueous Solubility Prediction Method
logp	1.948		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rhoc	268.43 ± 19.75	kg/m3	NIST Webbook
rhoc	268.43	kg/m3	NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	874.00		NIST Webbook

rinpol	875.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	879.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1308.00		NIST Webbook
tb	427.65 ± 2.00	K	NIST Webbook
tb	428.45 ± 1.00	K	NIST Webbook
tb	428.15 ± 3.00	K	NIST Webbook
tb	428.55 ± 2.00	K	NIST Webbook
tb	426.15 ± 3.00	K	NIST Webbook
tb	426.65 ± 1.50	K	NIST Webbook
tb	428.15 ± 2.00	K	NIST Webbook
tb	428.15 ± 3.00	K	NIST Webbook
tb	428.25 ± 0.50	K	NIST Webbook
tb	425.15 ± 3.00	K	NIST Webbook
tb	427.40 ± 2.00	K	NIST Webbook
tb	429.10 ± 1.00	K	NIST Webbook
tc	602.60	K	NIST Webbook

tc	602.60 ± 0.50	K	NIST Webbook
tc	602.60 ± 0.25	K	NIST Webbook
tf	231.55	K	Aqueous Solubility Prediction Method
tf	235.10	K	Calorimetric and FTIR study of selected aliphatic heptanols
vc	0.432	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method
cpg	269.25	J/mol×K	505.89	Joback Method
cpg	279.32	J/mol×K	533.18	Joback Method
cpg	289.00	J/mol×K	560.47	Joback Method
cpg	298.30	J/mol×K	587.77	Joback Method
cpg	307.23	J/mol×K	615.06	Joback Method
cpl	317.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0221021	Pa×s	253.94	Joback Method
dvisc	0.1594974	Pa×s	214.47	Joback Method
dvisc	0.0052125	Pa×s	293.41	Joback Method
dvisc	0.0017316	Pa×s	332.88	Joback Method
dvisc	0.0007266	Pa×s	372.36	Joback Method
dvisc	0.0003601	Pa×s	411.83	Joback Method
dvisc	0.0002018	Pa×s	451.30	Joback Method
hvapt	58.20	kJ/mol	374.00	NIST Webbook
hvapt	63.10	kJ/mol	301.00	NIST Webbook
hvapt	53.10	kJ/mol	388.50	NIST Webbook
hvapt	56.90	kJ/mol	374.00	NIST Webbook
pvap	0.03	kPa	282.43	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.03	kPa	282.95	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.03	kPa	283.15	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.06	kPa	288.83	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.07	kPa	291.38	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.08	kPa	292.57	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.08	kPa	293.13	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.10	kPa	295.02	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.12	kPa	297.63	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.13	kPa	297.95	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.13	kPa	298.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.18	kPa	302.40	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.18	kPa	302.65	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.19	kPa	302.91	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.20	kPa	303.51	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	0.28	kPa	307.75	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	0.28	kPa	307.77	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.43	kPa	313.62	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.69	kPa	320.38	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.70	kPa	320.38	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.00	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52932e+01
Coeff. B	-3.51406e+03
Coeff. C	-9.88080e+01
Temperature range (K), min.	332.99
Temperature range (K), max.	450.86

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589559&Units=SI
Vapour pressures and heat capacity measurements on the C7 C9 secondary aliphatic alcohols:	https://www.doi.org/10.1016/j.jct.2006.10.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Calorimetric and FTIR study of selected aliphatic heptanols:	https://www.doi.org/10.1016/j.fluid.2016.04.003
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576

Legend

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
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