

1-Heptanol

Other names:	1-Heptanol
	1-Heptyl alcohol
	1-Hydroxyheptane
	Alcohol C7
	Enanthic alcohol
	Enanthyl alcohol
	Gentanol
	Heptan-1-ol
	Heptane-1-ol
	Heptanol-1
	Heptyl alcohol
	Heptyl alcohol, n-
	NSC 3703
	l'Alcool n-heptylique primaire
	n-C7H15OH
	n-Heptan-1-ol
	n-Heptanol
	n-Heptanol-1
	n-Heptyl alcohol
Inchi:	InChI=1S/C7H16O/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3
InchiKey:	BBMCTIGTTCKYKF-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCCCCCO
Mol. weight [g/mol]:	116.20
CAS:	111-70-6

Physical Properties

Property code	Value	Unit	Source
af	0.5600		KDB
affp	799.00	kJ/mol	NIST Webbook
aigt	255.37	K	KDB
chl	-4638.01 ± 0.79	kJ/mol	NIST Webbook
chl	-4637.80 ± 0.50	kJ/mol	NIST Webbook
chl	-4642.52 ± 0.71	kJ/mol	NIST Webbook
chl	-4631.90	kJ/mol	NIST Webbook
chl	-4631.90 ± 2.30	kJ/mol	NIST Webbook
dm	1.70	debye	KDB

fpc	349.82	K	KDB
gf	-121.00	kJ/mol	KDB
hf	-332.00	kJ/mol	KDB
hfl	-403.20 ± 0.80	kJ/mol	NIST Webbook
hfl	-398.80 ± 0.84	kJ/mol	NIST Webbook
hfl	-460.40 ± 3.00	kJ/mol	NIST Webbook
hfl	-409.40 ± 2.30	kJ/mol	NIST Webbook
hfl	-403.40 ± 0.50	kJ/mol	NIST Webbook
hfus	17.97	kJ/mol	Joback Method
hvap	67.80 ± 1.50	kJ/mol	NIST Webbook
hvap	66.80 ± 0.20	kJ/mol	NIST Webbook
hvap	66.81 ± 0.20	kJ/mol	NIST Webbook
hvap	66.40	kJ/mol	NIST Webbook
hvap	66.50	kJ/mol	NIST Webbook
hvap	66.81	kJ/mol	NIST Webbook
hvap	67.10	kJ/mol	NIST Webbook
hvap	66.90 ± 0.40	kJ/mol	NIST Webbook
hvap	69.70	kJ/mol	NIST Webbook
ie	10.40 ± 0.10	eV	NIST Webbook
ie	9.84	eV	NIST Webbook
ie	10.35	eV	NIST Webbook
log10ws	-1.81		Aqueous Solubility Prediction Method
log10ws	-1.81		Estimated Solubility Method
logp	1.949		Crippen Method
mccvol	115.360	ml/mol	McGowan Method
pc	3060.00 ± 20.00	kPa	NIST Webbook
pc	3058.00 ± 20.00	kPa	NIST Webbook
pc	3058.00 ± 20.00	kPa	NIST Webbook
pc	3160.00 ± 50.00	kPa	NIST Webbook
pc	3058.00	kPa	KDB
rhoc	267.26 ± 3.49	kg/m3	NIST Webbook
rhoc	267.26 ± 2.32	kg/m3	NIST Webbook
rhoc	267.26	kg/m3	NIST Webbook
rhoc	266.10 ± 27.89	kg/m3	NIST Webbook
rinpol	970.00		NIST Webbook
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sg	485.80 ± 4.20	J/mol×K	NIST Webbook
sl	325.90	J/mol×K	NIST Webbook
tb	448.15 ± 2.00	K	NIST Webbook
tb	449.50	K	NIST Webbook
tb	447.30 ± 0.15	K	NIST Webbook
tb	449.55 ± 0.40	K	NIST Webbook
tb	446.15 ± 2.00	K	NIST Webbook
tb	448.95 ± 1.00	K	NIST Webbook
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tb	449.25 ± 0.50	K	NIST Webbook
tb	445.90 ± 1.00	K	NIST Webbook
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tb	448.15 ± 2.00	K	NIST Webbook
tb	449.05 ± 0.50	K	NIST Webbook
tb	448.75 ± 0.35	K	NIST Webbook
tc	632.60	K	KDB
tf	238.65	K	Aqueous Solubility Prediction Method
tf	238.25 ± 0.50	K	NIST Webbook
tf	238.60 ± 0.40	K	NIST Webbook
tf	239.00	K	KDB
tf	239.40 ± 0.50	K	NIST Webbook
tt	240.00 ± 0.20	K	NIST Webbook
vc	0.435	m3/kmol	KDB
vc	0.435	m3/kmol	NIST Webbook
zc	0.2529070		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.80	J/mol×K	451.74	Joback Method
cpg	258.38	J/mol×K	478.48	Joback Method
cpg	268.58	J/mol×K	505.23	Joback Method
cpg	278.39	J/mol×K	531.97	Joback Method
cpg	287.84	J/mol×K	558.71	Joback Method
cpg	296.94	J/mol×K	585.45	Joback Method
cpg	305.68	J/mol×K	612.20	Joback Method

cpl	270.80	J/mol×K	298.15	NIST Webbook
cpl	272.29	J/mol×K	298.15	NIST Webbook
cpl	297.00	J/mol×K	303.35	NIST Webbook
cpl	273.67	J/mol×K	298.15	NIST Webbook
cpl	278.90	J/mol×K	302.97	NIST Webbook
cpl	274.10	J/mol×K	298.00	NIST Webbook
cpl	278.57	J/mol×K	298.15	NIST Webbook
dvisc	0.0002110	Pa×s	451.74	Joback Method
dvisc	0.0132124	Pa×s	266.51	Joback Method
dvisc	0.0673608	Pa×s	229.47	Joback Method
dvisc	0.0014716	Pa×s	340.61	Joback Method
dvisc	0.0006783	Pa×s	377.65	Joback Method
dvisc	0.0003591	Pa×s	414.70	Joback Method
dvisc	0.0038567	Pa×s	303.56	Joback Method
hfust	18.35	kJ/mol	239.90	NIST Webbook
hfust	18.16	kJ/mol	240.40	NIST Webbook
hfust	18.16	kJ/mol	240.40	NIST Webbook
hfust	18.18	kJ/mol	240.40	NIST Webbook
hvapt	48.12	kJ/mol	449.10	KDB
hvapt	65.20	kJ/mol	310.50	NIST Webbook
hvapt	62.50	kJ/mol	392.50	NIST Webbook
hvapt	62.60	kJ/mol	393.00	NIST Webbook
hvapt	65.20	kJ/mol	391.00	NIST Webbook
hvapt	62.90	kJ/mol	379.00	NIST Webbook
rho1	822.00	kg/m3	293.00	KDB
sfust	75.60	J/mol×K	240.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46759e+01

Coeff. B	-3.44597e+03
Coeff. C	-1.05377e+02
Temperature range (K), min.	344.87
Temperature range (K), max.	473.36

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.98081e+02
Coeff. B	-1.56272e+04
Coeff. C	-2.63701e+01
Coeff. D	1.17680e-05
Temperature range (K), min.	239.15
Temperature range (K), max.	631.90

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111706&Units=SI
KDB Pure (Korean Thermophysical Properties Databank):	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=838
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=838
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=838
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment

dvisc:	Dynamic viscosity
fpc:	Flash Point (Closed Cup Method)
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
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
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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