Benzene, heptyl-

Other names:	1-PHENYLHEPTANE
	HEPTYLBENZENE
	Heptane, 1(or 7)-phenyl-
	Heptane, 1-phenyl-
	n-Heptylbenzene
Inchi:	InChI=1S/C13H20/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h6,8-9,11-12H,2-5,7,10H2,1H3
InchiKey:	LBNXAWYDQUGHGX-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	CCCCCCCc1ccccc1
Mol. weight [g/mol]:	176.30
CAS:	1078-71-3

Physical Properties

Property code	Value	Unit	Source
af	0.5300		KDB
gf	170.99	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	64.90	kJ/mol	NIST Webbook
hvap	64.20 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.37		Crippen Method
logp	4.200		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2200.00	kPa	KDB
rinpol	1369.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1362.93		NIST Webbook
rinpol	1351.94		NIST Webbook
rinpol	1349.17		NIST Webbook
rinpol	1344.62		NIST Webbook
rinpol	1367.67		NIST Webbook
rinpol	1370.87		NIST Webbook
rinpol	231.70		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1351.94		NIST Webbook
rinpol	1337.00		NIST Webbook

rinpol	231.70		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1349.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1612.00		NIST Webbook
tb	506.00 ± 4.00	K	NIST Webbook
tb	508.00 ± 6.00	K	NIST Webbook
tb	506.00 ± 6.00	K	NIST Webbook
tb	508.00 ± 5.00	K	NIST Webbook
tb	519.20	K	KDB
tb	513.00 ± 5.00	K	NIST Webbook
tb	506.20	K	NIST Webbook
tb	418.30 ± 0.60	K	NIST Webbook
tb	503.00 ± 5.00	K	NIST Webbook
tb	507.00 ± 6.00	K	NIST Webbook
tb	518.00 ± 6.00	K	NIST Webbook
tb	514.00 ± 6.00	K	NIST Webbook
tb	514.00 ± 5.00	K	NIST Webbook
tb	514.00 ± 5.00	K	NIST Webbook
tb	515.00 ± 4.00	K	NIST Webbook
tb	515.00 ± 6.00	K	NIST Webbook

tb	506.00 ± 6.00	K	NIST Webbook
tb	506.15 ± 3.00	K	NIST Webbook
tb	518.70	K	NIST Webbook
tc	713.50	K	KDB
tf	225.00	K	KDB
vc	0.660	m3/kmol	KDB
zc	0.2447570		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.80	J/mol×K	523.52	Joback Method
cpg	410.37	J/mol×K	556.29	Joback Method
cpg	427.01	J/mol×K	589.05	Joback Method
cpg	442.75	J/mol×K	621.82	Joback Method
cpg	457.64	J/mol×K	654.59	Joback Method
cpg	471.71	J/mol×K	687.36	Joback Method
cpg	484.99	J/mol×K	720.12	Joback Method
cpl	269.00	J/mol×K	294.00	NIST Webbook
dvisc	0.0038028	Pa×s	262.69	Joback Method
dvisc	0.0016294	Pa×s	306.16	Joback Method
dvisc	0.0008620	Pa×s	349.63	Joback Method
dvisc	0.0005250	Pa×s	393.11	Joback Method
dvisc	0.0003529	Pa×s	436.58	Joback Method
dvisc	0.0002549	Pa×s	480.05	Joback Method
dvisc	0.0001944	Pa×s	523.52	Joback Method
hvapt	45.19	kJ/mol	519.20	KDB
hvapt	54.00	kJ/mol	475.00	NIST Webbook
pvap	5.85e-03	kPa	300.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	3.47e-03	kPa	294.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

pvap	4.55e-03	kPa	297.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	2.86e-03	kPa	292.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	7.61e-03	kPa	303.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	9.55e-03	kPa	306.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.01	kPa	309.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.01	kPa	312.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.02	kPa	315.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.02	kPa	318.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.03	kPa	321.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

pvap	0.03	kPa	323.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.04	kPa	326.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.05	kPa	328.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.06	kPa	331.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.07	kPa	333.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.08	kPa	336.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.10	kPa	338.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	
pvap	0.11	kPa	341.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes	

pvap	0.13	kPa	343.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.16	kPa	346.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.18	kPa	348.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.22	kPa	351.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.25	kPa	353.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46941e+01
Coeff. B	-4.48052e+03
Coeff. C	-7.45680e+01
Temperature range (K), min.	385.57
Temperature range (K), max.	552.10

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	1.48905e+02
Coeff. B	-1.34446e+04
Coeff. C	-1.93270e+01
Coeff. D	9.07112e-06
Temperature range (K), min.	225.15
Temperature range (K), max.	714.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes between (332 and 401) K:	https://www.doi.org/10.1021/je050273f
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the linear n-alkylbenzenes:	https://www.doi.org/10.1016/j.jct.2005.11.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1078713&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=706
KDB:	https://www.cheric.org/files/research/kdb/mol/mol706.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility