Heptadecylbenzene

Other names:	1-phenylheptadecane
	benzene, heptadecyl-
	heptadecane, 1-phenyl-
Inchi:	InChI=1S/C23H40/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23-21-18-16-19-22-23/h1
InchiKey:	ZMPPFNHWXMJARX-UHFFFAOYSA-N
Formula:	C23H40
SMILES:	CCCCCCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	316.57
CAS:	14752-75-1

Physical Properties

Property code	Value	Unit	Source
af	0.9199		Cheméo Relay (1.0)
gf	255.19	kJ/mol	Joback Method
hf	-269.22	kJ/mol	Cheméo Relay (1.0)
hfus	49.37	kJ/mol	Joback Method
hvap	112.24	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-8.57		Cheméo Relay (1.0)
logp	8.101		Crippen Method
mcvol	311.170	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
tb	626.30	K	Cheméo Relay (1.0)
tc	809.40	K	Cheméo Relay (1.0)
tf	311.00 ± 2.00	K	NIST Webbook
vc	1.226	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.99	J/mol×K	904.62	Joback Method
cpg	1056.00	J/mol×K	935.08	Joback Method
cpg	966.62	J/mol×K	782.78	Joback Method
cpg	986.46	J/mol×K	813.24	Joback Method

cpg	1005.27	J/mol×K	843.70	Joback Method
cpg	1023.10	J/mol×K	874.16	Joback Method
cpg	945.69	J/mol×K	752.32	Joback Method
dvisc	0.0003574	Pa×s	501.03	Joback Method
dvisc	0.0007328	Pa×s	438.21	Joback Method
dvisc	0.0019107	Pa×s	375.39	Joback Method
dvisc	0.0002045	Pa×s	563.86	Joback Method
dvisc	0.0001309	Pa×s	626.68	Joback Method
dvisc	0.0000909	Pa×s	689.50	Joback Method
dvisc	0.0000671	Pa×s	752.32	Joback Method
hvapt	98.50	kJ/mol	539.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	292.80	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41856e+01
Coeff. B	-4.87150e+03
Coeff. C	-1.54932e+02
Temperature range (K), min.	505.45
Temperature range (K), max.	703.89

Datasets

Speed of sound, m/s

Pressure, kPa - Liquid	Temperature, K - Liquid	Speed of sound, m/s - Liquid
100.00	303.15	1422.6
100.00	313.15	1387.1
100.00	323.15	1352.6
100.00	333.15	1319.9
100.00	343.15	1287.0
100.00	353.15	1255.2
100.00	363.15	1223.6
100.00	373.15	1193.0
10000.00	303.15	1467.5
10000.00	313.15	1433.6
10000.00	323.15	1402.3
10000.00	333.15	1370.2
10000.00	343.15	1338.7
10000.00	353.15	1308.6
10000.00	363.15	1278.7
10000.00	373.15	1249.5
20000.00	303.15	1510.9
20000.00	313.15	1479.2
20000.00	323.15	1447.9
20000.00	333.15	1417.3
20000.00	343.15	1387.3
20000.00	353.15	1359.3
20000.00	363.15	1330.3
20000.00	373.15	1302.6
30000.00	303.15	1552.0
30000.00	313.15	1520.4
30000.00	323.15	1490.8
30000.00	333.15	1461.4
30000.00	343.15	1432.3
30000.00	353.15	1405.3
30000.00	363.15	1378.0
30000.00	373.15	1351.4
40000.00	303.15	1590.5
40000.00	313.15	1559.7
40000.00	323.15	1531.1
40000.00	333.15	1502.9
40000.00	343.15	1475.5
40000.00	353.15	1448.5
40000.00	363.15	1422.2

40000.00	373.15	1396.8
50000.00	303.15	1627.2
50000.00	313.15	1597.9
50000.00	323.15	1569.2
50000.00	333.15	1542.1
50000.00	343.15	1515.3
50000.00	353.15	1489.5
50000.00	363.15	1464.0
50000.00	373.15	1439.2
60000.00	303.15	1661.9
60000.00	313.15	1633.6
60000.00	323.15	1605.8
60000.00	333.15	1579.2
60000.00	343.15	1553.3
60000.00	353.15	1528.3
60000.00	363.15	1503.3
60000.00	373.15	1479.7
70000.00	303.15	1695.6
70000.00	313.15	1667.3
70000.00	323.15	1640.7
70000.00	333.15	1614.6
70000.00	343.15	1589.5
70000.00	353.15	1564.8
70000.00	363.15	1541.1
70000.00	373.15	1517.7
80000.00	313.15	1700.0
80000.00	323.15	1673.9
80000.00	333.15	1648.7
80000.00	343.15	1624.1
80000.00	353.15	1600.1
80000.00	363.15	1576.4
80000.00	373.15	1553.8
90000.00	313.15	1731.8
90000.00	323.15	1705.8
90000.00	333.15	1681.3
90000.00	343.15	1657.2
90000.00	353.15	1633.4
90000.00	363.15	1610.7
90000.00	373.15	1588.6
100000.00	313.15	1762.0
100000.00	323.15	1736.6
100000.00	333.15	1712.2
100000.00	343.15	1688.0
100000.00	353.15	1665.5

100000.00	363.15	1643.4
100000.00	373.15	1621.8
110000.00	313.15	1790.2
110000.00	323.15	1766.3
110000.00	333.15	1742.3
110000.00	343.15	1719.2
110000.00	353.15	1696.9
110000.00	363.15	1674.6
110000.00	373.15	1653.6
120000.00	313.15	1818.7
120000.00	323.15	1794.9
120000.00	333.15	1771.7
120000.00	343.15	1748.7
120000.00	353.15	1726.9
120000.00	363.15	1705.0
120000.00	373.15	1684.3
130000.00	313.15	1847.1
130000.00	323.15	1822.8
130000.00	333.15	1799.8
130000.00	343.15	1777.4
130000.00	353.15	1755.8
130000.00	363.15	1734.4
130000.00	373.15	1713.8
140000.00	323.15	1849.3
140000.00	333.15	1826.9
140000.00	343.15	1805.0
140000.00	353.15	1783.8
140000.00	363.15	1763.3
140000.00	373.15	1742.7
150000.00	323.15	1875.5
150000.00	333.15	1853.6
150000.00	343.15	1832.0
150000.00	353.15	1811.1
150000.00	363.15	1790.0
150000.00	373.15	1770.5

Reference *https://www.doi.org/10.1021/je049973v*

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:	https://www.doi.org/10.1021/je700529y
Speed of Sound, Density, and Compressibility of Alkyl-Benzenes as a Function of Pressure and Temperature:	https://www.doi.org/10.1021/je049973v
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14752751&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/73-686-0/Heptadecylbenzene.pdf
Generated by Cheméo on 2026-07-21 13:08:01.194272794 +0000 UTC m=+150377.036158185.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.