Benzene, octadecyl-

Other names:	1-Phenyloctadecane
	2-Phenyloctadecane
	Octadecane, 1-phenyl-
	Octadecylbenzene
	n-Octadecylbenzene
Inchi:	InChI=1S/C24H42/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-21-24-22-19-17-20-23-24
InchiKey:	WSVDSBZMYJJMSB-UHFFFAOYSA-N
Formula:	C24H42
SMILES:	CCCCCCCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	330.59
CAS:	4445-07-2

Physical Properties

Property code	Value	Unit	Source
gf	263.61	kJ/mol	Joback Method
hf	-302.16	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.491		Crippen Method
mcvol	325.260	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	2509.10		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2494.30		NIST Webbook
ripol	2712.90		NIST Webbook
ripol	2712.90		NIST Webbook
tb	775.20	K	Joback Method
tc	958.96	K	Joback Method
tf	308.65 ± 2.00	K	NIST Webbook
tf	302.15 ± 3.00	K	NIST Webbook
tf	309.00 ± 3.00	K	NIST Webbook
tf	308.15 ± 2.00	K	NIST Webbook
tf	308.65 ± 2.00	K	NIST Webbook
tf	306.00 ± 1.50	K	NIST Webbook
tf	298.65 ± 3.00	K	NIST Webbook
tf	303.15 ± 2.00	K	NIST Webbook

tf	309.65 ± 1.00	K	NIST Webbook
tf	308.00 ± 3.00	K	NIST Webbook
tf	308.65 ± 2.00	K	NIST Webbook
tf	308.70 ± 2.00	K	NIST Webbook
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.10	J/mol×K	775.20	Joback Method
cpg	1028.27	J/mol×K	805.83	Joback Method
cpg	1048.34	J/mol×K	836.45	Joback Method
cpg	1067.36	J/mol×K	867.08	Joback Method
cpg	1085.38	J/mol×K	897.70	Joback Method
cpg	1102.45	J/mol×K	928.33	Joback Method
cpg	1118.63	J/mol×K	958.96	Joback Method
dvisc	0.0017168	Pa×s	386.66	Joback Method
dvisc	0.0006534	Pa×s	451.42	Joback Method
dvisc	0.0003169	Pa×s	516.17	Joback Method
dvisc	0.0001806	Pa×s	580.93	Joback Method
dvisc	0.0001152	Pa×s	645.69	Joback Method
dvisc	0.0000798	Pa×s	710.44	Joback Method
dvisc	0.0000587	Pa×s	775.20	Joback Method
hvapt	101.00	kJ/mol	549.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	307.90	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	312.50	K	20100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

tfp	319.50	K	50300.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	324.50	K	74900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	329.50	K	99600.00	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	1.39373e+01
Coeff. B	-4.75677e+03
Coeff. C	-1.65703e+02
Temperature range (K), min.	514.19
Temperature range (K), max.	717.16

Datasets

Speed of sound, m/s

Pressure, kPa - Liquid	Temperature, K - Liquid	Speed of sound, m/s - Liquid
100.00	313.15	1392.9
100.00	323.15	1357.8
100.00	333.15	1325.5
100.00	343.15	1292.7
100.00	353.15	1260.7
100.00	363.15	1229.5
100.00	373.15	1198.7
10000.00	313.15	1439.6

10000.00	323.15	1406.8
10000.00	333.15	1374.8
10000.00	343.15	1344.1
10000.00	353.15	1313.4
10000.00	363.15	1284.8
10000.00	373.15	1255.2
20000.00	313.15	1484.1
20000.00	323.15	1452.4
20000.00	333.15	1422.6
20000.00	343.15	1392.8
20000.00	353.15	1364.1
20000.00	363.15	1334.9
20000.00	373.15	1308.3
30000.00	313.15	1525.8
30000.00	323.15	1495.5
30000.00	333.15	1466.1
30000.00	343.15	1437.7
30000.00	353.15	1410.0
30000.00	363.15	1382.7
30000.00	373.15	1356.6
40000.00	313.15	1564.8
40000.00	323.15	1535.6
40000.00	333.15	1507.5
40000.00	343.15	1480.2
40000.00	353.15	1454.0
40000.00	363.15	1427.1
40000.00	373.15	1401.7
50000.00	313.15	1602.4
50000.00	323.15	1574.0
50000.00	333.15	1546.7
50000.00	343.15	1519.9
50000.00	353.15	1494.4
50000.00	363.15	1469.1
50000.00	373.15	1444.5
60000.00	313.15	1638.1
60000.00	323.15	1610.3
60000.00	333.15	1583.5
60000.00	343.15	1558.1
60000.00	353.15	1532.6
60000.00	363.15	1508.3
60000.00	373.15	1484.7
70000.00	313.15	1672.1
70000.00	323.15	1645.1
70000.00	333.15	1619.1

70000.00	343.15	1594.2
70000.00	353.15	1569.2
70000.00	363.15	1545.7
70000.00	373.15	1522.0
80000.00	313.15	1704.7
80000.00	323.15	1678.7
80000.00	333.15	1652.8
80000.00	343.15	1628.6
80000.00	353.15	1604.3
80000.00	363.15	1581.7
80000.00	373.15	1558.6
90000.00	323.15	1710.4
90000.00	333.15	1685.7
90000.00	343.15	1661.5
90000.00	353.15	1638.2
90000.00	363.15	1615.7
90000.00	373.15	1592.9
100000.00	323.15	1741.3
100000.00	333.15	1717.0
100000.00	343.15	1693.1
100000.00	353.15	1670.3
100000.00	363.15	1648.3
100000.00	373.15	1626.3
110000.00	323.15	1771.2
110000.00	333.15	1747.3
110000.00	343.15	1723.6
110000.00	353.15	1701.4
110000.00	363.15	1679.8
110000.00	373.15	1657.9
120000.00	323.15	1799.2
120000.00	333.15	1775.7
120000.00	343.15	1753.5
120000.00	353.15	1731.3
120000.00	363.15	1710.0
120000.00	373.15	1688.5
130000.00	333.15	1803.9
130000.00	343.15	1781.9
130000.00	353.15	1759.9
130000.00	363.15	1739.2
130000.00	373.15	1718.7
140000.00	333.15	1830.9
140000.00	343.15	1809.4
140000.00	353.15	1788.8
140000.00	363.15	1767.5

140000.00	373.15	1746.6
150000.00	333.15	1857.5
150000.00	343.15	1836.3
150000.00	353.15	1815.1
150000.00	363.15	1795.5
150000.00	373.15	1774.6

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Speed of Sound, Density, and Compressibility of Alkyl-Benzenes as a Function of Pressure and Temperature:	https://www.doi.org/10.1021/je049973v
Solid-Liquid Equilibria under High Pressure of Nine Pure Alkanes:	https://www.doi.org/10.1021/je700529y
Heptadecylbenzene and Octadecylbenzene:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4445072&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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
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