Benzene, octyl-

Other names: 1-PHENYLOCTANE
Octane, 1-phenyl-
Octylbenzene
PHENYLOCTANE
n-Octylbenzene
Inchi: InChI=1S/C14H22/c1-2-3-4-5-6-8-11-14-12-9-7-10-13-14/h7,9-10,12-13H,2-6,8,11H2,1H
InchiKey: CDKDZKXSXLNROY-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCCCCCc1ccccc1
Mol. weight [g/mol]: 190.32
CAS: 2189-60-8

Physical Properties

Property code	Value	Unit	Source
af	0.5770		KDB
gf	179.41	kJ/mol	Joback Method
hf	-95.76	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.590		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2040.00	kPa	KDB
rinpol	1453.00		NIST Webbook
rinpol	1475.03		NIST Webbook
rinpol	1465.10		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1466.50		NIST Webbook
rinpol	249.10		NIST Webbook
rinpol	249.10		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1448.08		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1451.00		NIST Webbook

rinpol	1466.50		NIST Webbook
rinpol	1466.30		NIST Webbook
rinpol	1461.60		NIST Webbook
rinpol	1466.50		NIST Webbook
rinpol	1468.20		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1455.20		NIST Webbook
rinpol	1461.60		NIST Webbook
rinpol	1466.50		NIST Webbook
rinpol	1468.20		NIST Webbook
rinpol	1466.50		NIST Webbook
rinpol	1466.30		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1480.30		NIST Webbook
rinpol	1465.10		NIST Webbook
rinpol	1474.20		NIST Webbook
rinpol	1484.10		NIST Webbook
rinpol	1471.70		NIST Webbook
rinpol	1478.30		NIST Webbook
rinpol	1448.08		NIST Webbook
rinpol	1452.71		NIST Webbook
rinpol	1455.83		NIST Webbook
rinpol	1466.64		NIST Webbook
rinpol	1471.90		NIST Webbook
rinpol	1475.03		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1456.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1715.00		NIST Webbook
tb	529.65 ± 2.50	K	NIST Webbook
tb	537.70	K	NIST Webbook
tb	535.20	K	NIST Webbook
tb	527.00 ± 6.00	K	NIST Webbook
tb	531.00 ± 6.00	K	NIST Webbook
tb	535.00 ± 7.00	K	NIST Webbook

tb	537.60	K	KDB
tb	538.00 ± 2.00	K	NIST Webbook
tb	538.00 ± 5.00	K	NIST Webbook
tb	536.00 ± 5.00	K	NIST Webbook
tb	530.00 ± 5.00	K	NIST Webbook
tb	536.00 ± 7.00	K	NIST Webbook
tc	728.00	K	KDB
tf	237.00	K	KDB
vc	0.720	m3/kmol	KDB
zc	0.2426580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.27	J/mol×K	740.42	Joback Method
cpg	508.93	J/mol×K	675.75	Joback Method
cpg	493.52	J/mol×K	643.41	Joback Method
cpg	477.23	J/mol×K	611.07	Joback Method
cpg	460.03	J/mol×K	578.74	Joback Method
cpg	441.87	J/mol×K	546.40	Joback Method
cpg	523.51	J/mol×K	708.08	Joback Method
cpl	291.00	J/mol×K	295.00	NIST Webbook
dvisc	0.0015666	Pa×s	319.37	Joback Method
dvisc	0.0008196	Pa×s	364.77	Joback Method
dvisc	0.0004949	Pa×s	410.18	Joback Method
dvisc	0.0003305	Pa×s	455.59	Joback Method
dvisc	0.0002374	Pa×s	500.99	Joback Method
dvisc	0.0037116	Pa×s	273.96	Joback Method
dvisc	0.0001802	Pa×s	546.40	Joback Method
hfust	29.96	kJ/mol	234.20	NIST Webbook
hfust	29.96	kJ/mol	234.20	NIST Webbook
hfust	29.96	kJ/mol	234.20	NIST Webbook
hvapt	63.10	kJ/mol	384.00	NIST Webbook
hvapt	67.40	kJ/mol	377.50	NIST Webbook
hvapt	46.86	kJ/mol	537.60	KDB
hvapt	66.20	kJ/mol	357.50	NIST Webbook

srf	0.03	N/m	293.90	Densities and Viscosities at 293.15 373.15 K, Speeds of Sound and Bulk Moduli at 293.15 333.15 K, Surface Tensions, and Flash Points of Binary Mixtures of n-Hexadecane and Alkylbenzenes at 0.1 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51719e+01
Coeff. B	-4.88461e+03
Coeff. C	-7.11620e+01
Temperature range (K), min.	399.33
Temperature range (K), max.	566.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.15260e+02
Coeff. B	-1.23375e+04
Coeff. C	-1.41827e+01
Coeff. D	5.11526e-06
Temperature range (K), min.	237.15
Temperature range (K), max.	729.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities and Viscosities at 293.15 373.15 K, Speeds of Sound and Bulk Moduli at 293.15 333.15 K, Surface Tensions, and Flash Points of Binary Mixtures of n-Hexadecane and Alkylbenzenes at 0.1 MPa:	https://www.doi.org/10.1021/acs.jced.7b00087
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol707.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Fluid phase equilibria in the binary system trifluoromethane + 1-phenyloctane:	https://www.doi.org/10.1016/j.fluid.2010.04.013
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=707
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2189608&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility