Benzene, dodecyl-

Other names:	1-Dodecylbenzene
	1-PHENYLDODECANE
	ALKYLATE P 1
	Detergent Alkylate No. 2
	Detergent alkylate
	Dodecane, 1-phenyl-
	Dodecylbenzene
	LAURYLBENZENE
	Marlican
	NSC 102805
	Nalkylene 500
	Phenyldodecan
	Phenyldodecane
	n-Dodecylbenzene
Inchi:	InChI=1S/C18H30/c1-2-3-4-5-6-7-8-9-10-12-15-18-16-13-11-14-17-18/h11,13-14,16-17H
InchiKey:	KWKXNDCHNDYVRT-UHFFFAOYSA-N
Formula:	C18H30
SMILES:	CCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	246.43
CAS:	123-01-3

Physical Properties

Property code	Value	Unit	Source
af	0.7730		KDB
gf	213.09	kJ/mol	Joback Method
hf	-178.32	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hsub	135.10	kJ/mol	NIST Webbook
hvap	89.60	kJ/mol	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-6.46		Crippen Method
logp	6.150		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1580.00	kPa	KDB
rinpol	1872.60		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1878.00		NIST Webbook

rinpol	1870.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1872.60		NIST Webbook
rinpol	1866.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2155.00		NIST Webbook
tb	590.00 ± 5.00	K	NIST Webbook
tb	600.80	K	KDB
tc	774.00	K	KDB
tf	266.00 ± 2.00	K	NIST Webbook
tf	270.00 ± 2.00	K	NIST Webbook
tf	276.00	K	KDB
vc	0.980	m3/kmol	KDB
zc	0.2406050		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.40	J/mol×K	637.92	Joback Method
cpg	691.87	J/mol×K	699.76	Joback Method
cpg	757.49	J/mol×K	823.44	Joback Method
cpg	709.62	J/mol×K	730.68	Joback Method
cpg	726.46	J/mol×K	761.60	Joback Method
cpg	742.40	J/mol×K	792.52	Joback Method
cpg	673.14	J/mol×K	668.84	Joback Method
dvisc	0.0001642	Pa×s	584.77	Joback Method
dvisc	0.0002326	Pa×s	531.63	Joback Method
dvisc	0.0003562	Pa×s	478.48	Joback Method
dvisc	0.0006066	Pa×s	425.33	Joback Method
dvisc	0.0012027	Pa×s	372.19	Joback Method
dvisc	0.0001228	Pa×s	637.92	Joback Method
dvisc	0.0029955	Pa×s	319.04	Joback Method
hfust	43.10	kJ/mol	274.60	NIST Webbook
hvapt	83.20	kJ/mol	393.00	NIST Webbook
hvapt	80.60	kJ/mol	396.00	NIST Webbook
hvapt	67.40	kJ/mol	552.50	NIST Webbook
hvapt	92.00	kJ/mol	275.00	NIST Webbook
hvapt	54.39	kJ/mol	600.80	KDB

srf	0.03	N/m	294.30	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	269.70	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	274.40	K	20200.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	279.00	K	40100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	283.40	K	60000.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	287.80	K	79900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	292.00	K	100000.00	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	1.52577e+01
Coeff. B	-5.30559e+03
Coeff. C	-1.02085e+02
Temperature range (K), min.	456.15
Temperature range (K), max.	635.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.68186e+02
Coeff. B	-2.21930e+04
Coeff. C	-3.63255e+01
Coeff. D	1.59623e-05
Temperature range (K), min.	275.93
Temperature range (K), max.	774.26

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Densities and Viscosities at 293.15 373.15 K, Speeds of Sound and Bulk Modulus at 293.15–373.15 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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=716
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123013&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol716.mol
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
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
tfp:	Melting point
vc:	Critical Volume
zc:	Critical Compressibility