Benzene, tridecyl-

Other names:	1-PHENYLTRIDECANE
	Detergent Alkylate No. 5
	TRIDANE
	Tridecane, 1-phenyl-
	Tridecylbenzene
	n-Tridecylbenzene
Inchi:	InChI=1S/C19H32/c1-2-3-4-5-6-7-8-9-10-11-13-16-19-17-14-12-15-18-19/h12,14-15,17-1
InchiKey:	MCVUKOYZUCWLQQ-UHFFFAOYSA-N
Formula:	C19H32
SMILES:	CCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	260.46
CAS:	123-02-4

Physical Properties

Property code	Value	Unit	Source
af	0.8160		KDB
gf	221.51	kJ/mol	Joback Method
hf	-198.96	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	94.60	kJ/mol	NIST Webbook
log10ws	-6.88		Crippen Method
logp	6.540		Crippen Method
mcvol	254.810	ml/mol	McGowan Method
pc	1500.00	kPa	KDB
rinpol	1971.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	1978.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2277.00		NIST Webbook
tb	614.40	K	KDB
tc	784.00	K	KDB
tf	283.00	K	KDB
vc	1.040	m3/kmol	KDB
zc	0.2393160		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.88	J/mol×K	814.22	Joback Method
cpg	766.64	J/mol×K	752.85	Joback Method
cpg	748.64	J/mol×K	722.17	Joback Method
cpg	729.65	J/mol×K	691.48	Joback Method
cpg	709.65	J/mol×K	660.80	Joback Method
cpg	783.71	J/mol×K	783.54	Joback Method
cpg	815.19	J/mol×K	844.91	Joback Method
dvisc	0.0027746	Pa×s	330.31	Joback Method
dvisc	0.0001098	Pa×s	660.80	Joback Method
dvisc	0.0001473	Pa×s	605.72	Joback Method
dvisc	0.0002095	Pa×s	550.64	Joback Method
dvisc	0.0003222	Pa×s	495.56	Joback Method
dvisc	0.0005518	Pa×s	440.47	Joback Method
dvisc	0.0011025	Pa×s	385.39	Joback Method
hvapt	90.00	kJ/mol	403.00	NIST Webbook
hvapt	56.07	kJ/mol	614.40	KDB
hvapt	72.00	kJ/mol	562.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	272.80	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	277.30	K	20100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	281.60	K	40300.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

tfp	285.90	K	60800.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	289.80	K	79900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	293.70	K	100100.00	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	1.56301e+01
Coeff. B	-5.56665e+03
Coeff. C	-1.06350e+02
Temperature range (K), min.	469.17
Temperature range (K), max.	645.82

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.89788e+02
Coeff. B	-2.39686e+04
Coeff. C	-3.93295e+01
Coeff. D	1.67783e-05
Temperature range (K), min.	283.15
Temperature range (K), max.	783.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol717.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123024&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=717
Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:	https://www.doi.org/10.1021/je700529y
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tfp:	Melting point
vc:	Critical Volume
zc:	Critical Compressibility