Benzene, hexadecyl-

Other names:	1-Phenylhexadecane
	Hexadecane, 1(or 16)-phenyl-
	Hexadecane, 1-phenyl-
	Hexadecylbenzene
	Phenyl hexadecane
	n-Hexadecylbenzene
Inchi:	InChI=1S/C22H38/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-19-22-20-17-15-18-21-22/h15,1
InchiKey:	DEQLTFPCJRGSHW-UHFFFAOYSA-N
Formula:	C22H38
SMILES:	CCCCCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	302.54
CAS:	1459-09-2

Physical Properties

Property code	Value	Unit	Source
gf	246.77	kJ/mol	Joback Method
hf	-260.88	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.710		Crippen Method
mcvol	297.080	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
rinpol	2292.10		NIST Webbook
rinpol	2306.70		NIST Webbook
ripol	2514.70		NIST Webbook
tb	729.44	K	Joback Method
tc	911.79	K	Joback Method
tf	295.15 ± 3.00	K	NIST Webbook
tf	300.00 ± 2.00	K	NIST Webbook
tf	300.00 ± 2.00	K	NIST Webbook
tf	313.55 ± 5.00	K	NIST Webbook
tf	300.00 ± 4.00	K	NIST Webbook
tf	280.20 ± 8.00	K	NIST Webbook
tf	280.00 ± 3.00	K	NIST Webbook

tf	298.00 ± 4.00	K	NIST Webbook
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.33	J/mol×K	911.79	Joback Method
cpg	978.49	J/mol×K	881.40	Joback Method
cpg	961.76	J/mol×K	851.01	Joback Method
cpg	944.11	J/mol×K	820.61	Joback Method
cpg	925.50	J/mol×K	790.22	Joback Method
cpg	905.87	J/mol×K	759.83	Joback Method
cpg	885.17	J/mol×K	729.44	Joback Method
dvisc	0.0021159	Pa×s	364.12	Joback Method
dvisc	0.0000763	Pa×s	729.44	Joback Method
dvisc	0.0001032	Pa×s	668.55	Joback Method
dvisc	0.0001482	Pa×s	607.67	Joback Method
dvisc	0.0002307	Pa×s	546.78	Joback Method
dvisc	0.0004013	Pa×s	485.89	Joback Method
dvisc	0.0008180	Pa×s	425.01	Joback Method
hvapt	79.50	kJ/mol	596.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	299.50	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	304.20	K	20000.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	308.60	K	40300.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

tfp	312.60	K	59900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	316.80	K	80400.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	320.90	K	100700.00	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	1.60085e+01
Coeff. B	-6.25440e+03
Coeff. C	-1.02598e+02
Temperature range (K), min.	500.44
Temperature range (K), max.	687.28

Sources

Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:	https://www.doi.org/10.1021/je700529y
Solubility and Miscibility for the Mixture of (Ethyl Fluoride + Alkylbenzene Oil):	https://www.doi.org/10.1021/je500075h
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=C1459092&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes between (332 and 401) K:	https://www.doi.org/10.1021/je050273f
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume