

# Benzene, pentadecyl-

**Other names:**

1-Phenylpentadecane  
Pentadecane, 1-phenyl-  
Pentadecylbenzene  
n-Pentadecylbenzene

**Inchi:**

InChI=1S/C21H36/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21-19-16-14-17-20-21/h14,16-1

**InchiKey:**

JIRNEODMTPGRGV-UHFFFAOYSA-N

**Formula:**

C<sub>21</sub>H<sub>36</sub>

**SMILES:**

CCCCCCCCCCCCCCCCc1ccccc1

**Mol. weight [g/mol]:**

288.51

**CAS:**

2131-18-2

## Physical Properties

Property code	Value	Unit	Source
gf	238.35	kJ/mol	Joback Method
hf	-240.24	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.320		Crippen Method
mcvol	282.990	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
tb	706.56	K	Joback Method
tc	889.03	K	Joback Method
tf	352.85	K	Joback Method
vc	1.103	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.61	J/mol×K	706.56	Joback Method
cpg	846.08	J/mol×K	736.97	Joback Method
cpg	865.51	J/mol×K	767.38	Joback Method
cpg	883.93	J/mol×K	797.79	Joback Method
cpg	901.40	J/mol×K	828.21	Joback Method

cpg	917.95	J/molxK	858.62	Joback Method
cpg	933.63	J/molxK	889.03	Joback Method
dvisc	0.0023303	Paxs	352.85	Joback Method
dvisc	0.0009087	Paxs	411.80	Joback Method
dvisc	0.0004486	Paxs	470.75	Joback Method
dvisc	0.0002591	Paxs	529.70	Joback Method
dvisc	0.0001671	Paxs	588.66	Joback Method
dvisc	0.0001167	Paxs	647.61	Joback Method
dvisc	0.0000865	Paxs	706.56	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	285.10	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	289.70	K	21000.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	294.10	K	40100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	298.40	K	59900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	302.80	K	80400.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	306.70	K	100200.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

## Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.59172e+01
Coeff. B	-6.09906e+03
Coeff. C	-9.90840e+01
Temperature range (K), min.	489.31
Temperature range (K), max.	674.16

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Solid-Liquid Equilibria under High Pressure of Nine Pure Aromatic Hydrocarbons:</b>	<a href="https://www.doi.org/10.1021/je700529y">https://www.doi.org/10.1021/je700529y</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131182&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>d<sub>visc</sub>:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tfp:</b>	Melting point
<b>vc:</b>	Critical Volume

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