

# 1-n-butylpyrene

**Other names:** Pyrene, 1-butyl.

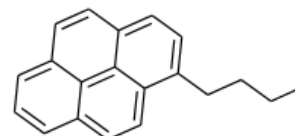
**InChI:** InChI=1S/C20H18/c1-2-3-5-14-8-9-17-11-10-15-6-4-7-16-12-13-18(14)20(17)19(15)16/h4,6-13H,2-3,5H2,1H3

**InChI Key:** UFOTZLIYHMGVAV-UHFFFAOYSA-N

**Formula:** C<sub>20</sub>H<sub>18</sub>

**SMILES:** CCCc1ccc2ccc3ccccc4ccc1c2c34

**Molecular Weight:** 258.36



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	515.23	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	273.74	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	34.46	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	68.66	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.93		Crippen Method
$P_c$	2060.49	kPa	Joback Method
$T_{\text{boil}}$	747.86	K	Joback Method
$T_c$	983.69	K	Joback Method
$T_{\text{fus}}$	483.52	K	Joback Method
$V_c$	0.84	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	591.79	J/mol×K	747.86	Joback Method
$\eta$	0.00	Paxs	747.86	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H18/c1-2-3-5-14-8-9-17-11-10-15-6-4-7-16-12-13-18\(14\)20\(17\)19\(15\)16/h4,6-13H,2-3,5H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H18/c1-2-3-5-14-8-9-17-11-10-15-6-4-7-16-12-13-18(14)20(17)19(15)16/h4,6-13H,2-3,5H2,1H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p,gas}$ : Ideal gas heat capacity (J/molxK).

$\eta$ : Dynamic viscosity (Pa $\times$ s).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

Latest version available from:

<https://www.cheméo.com/cid/35-859-0/1-n-butylpyrene>

Generated by Cheméo on Fri, 25 May 2018 22:24:01 +0000.

**Cheméo** (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.