

1-n-butylpyrene

Other names: Pyrene, 1-butyl.

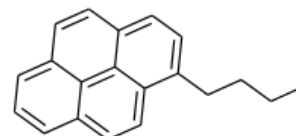
InChI: InChI=1S/C20H18/c1-2-3-5-14-8-9-17-11-10-15-6-4-7-16-12-13-18(14)20(17)19(15)16/h4,6-13H,2-3,5H2,1H3

InChI Key: UFOTZLIYHMGVAV-UHFFFAOYSA-N

Formula: C₂₀H₁₈

SMILES: CCCc1ccc2ccc3cccc4ccc1c2c34

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_{boil}	747.86	K	Joback Method
T_c	983.69	K	Joback Method
T_{fus}	483.52	K	Joback Method
V_c	0.84	m ³ /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
η	0.00	Paxs	747.86	Joback Method

Sources

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).

η : 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 (m³/kg-mol).

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