1-n-butylpyrene

Other names: Pyrene, 1-butyl.

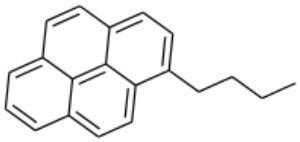
InChI: InChI=1S/C20H18/c1-2-3-5-14-8-9-17-11-10-15-6-4-7-16-12-13-18(14)20(17)19(15)16/h4,6-13H,2-3,5H2,1H3

InChI Key: UFOTZLIYHMGVAV-UHFFFAOYSA-N

Formula: C20H18

SMILES: CCCCc1ccc2ccc3cccc4ccc1c2c34

Molecular Weight: 258.36



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	515.23	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	273.74	kJ/mol	Joback Method
$\Delta_{fus} H°$	34.46	kJ/mol	Joback Method
$\Delta_{vap} H°$	68.66	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	591.79	J/mol×K	747.86	Joback Method
η	0.00	Pa×s	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).