Phenanthridine

Other names: 3,4-Benzoisoquinoline; 3,4-Benzoquinoline; 6-Phenanthridine; 9-Azaphenanthrene; Benzo[c]quinoline.

InChI: InChI=1S/C13H9N/c1-2-6-11-10(5-1)9-14-13-8-4-3-7-12(11)13/h1-9H

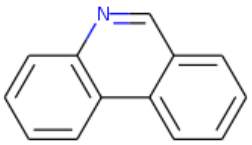
InChI Key: RDOWQLZANAYVLL-UHFFFAOYSA-N

Formula: C13H9N

SMILES: c1ccc2c(c1)cnc1ccccc12

Molecular Weight: 179.22

CAS: 229-87-8



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-6542.80 ± 1.20	kJ/mol	NIST Webbook
$\Delta_f H°_{gas}$	240.50 ± 4.20	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	141.90 ± 1.40	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	98.60 ± 4.00	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	98.60	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	98.60	kJ/mol	NIST Webbook
IE	8.31 ± 0.02	eV	NIST Webbook
IE	8.40 ± 0.10	eV	NIST Webbook
$logP_{oct/wat}$	3.39		Crippen Method
$S°_{solid,1\ bar}$	205.91	J/mol×K	NIST Webbook
$S°_{solid,1\ bar}$	205.91	J/mol×K	NIST Webbook
$S°_{solid,1\ bar}$	205.87	J/mol×K	NIST Webbook
T_{boil}	622.20	K	NIST Webbook
T_{fus}	379.40 ± 1.00	K	NIST Webbook
T_{fus}	379.65 ± 1.00	K	NIST Webbook
T_{fus}	379.65 ± 1.50	K	NIST Webbook
T_{fus}	372.65 ± 2.00	K	NIST Webbook

Property	Value	Unit	Source
T_{fus}	377.00 ± 2.00	K	NIST Webbook
T_{triple}	379.94 ± 0.02	K	NIST Webbook
T_{triple}	379.74 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,solid}$	201.87	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	201.87	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	201.79	J/mol×K	298.15	NIST Webbook
$\Delta_{fus}H$	0.02	kJ/mol	354.0	NIST Webbook
$\Delta_{fus}H$	22.83	kJ/mol	379.7	NIST Webbook
$\Delta_{sub}H$	100.00 ± 10.00	kJ/mol	305.5	NIST Webbook
$\Delta_{sub}H$	95.00 ± 4.00	kJ/mol	305.5	NIST Webbook
$\Delta_{vap}H$	74.30 ± 0.10	kJ/mol	428.0	NIST Webbook
$\Delta_{vap}H$	71.60 ± 0.10	kJ/mol	428.0	NIST Webbook
$\Delta_{vap}H$	68.90 ± 0.10	kJ/mol	428.0	NIST Webbook
$\Delta_{fus}S$	0.06	J/mol×K	354.0	NIST Webbook
$\Delta_{fus}S$	60.12	J/mol×K	379.7	NIST Webbook

Sources

NIST Webbook:
http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H9N/c1-2-6-11-10(5-1)9-14-13-8-4-3-7-12(11)13/h1-9H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
$C_{p,solid}$: Solid phase heat capacity (J/mol×K).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

Δ_f**H°**$_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).
***log*P**$_{oct/wat}$: Octanol/Water partition coefficient .
Δ_{fus}**S**: Entropy of fusion at a given temperature (J/mol×K).
S°$_{solid,1\ bar}$: Solid phase molar entropy at standard conditions (J/mol×K).
T$_{boil}$: Normal Boiling Point Temperature (K).
T$_{fus}$: Normal melting (fusion) point (K).
T$_{triple}$: Triple Point Temperature (K).

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