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
InchiKey:	RDOWQLZANAYVLL-UHFFFAOYSA-N
Formula:	C13H9N
SMILES:	c1ccc2c(c1)cnc1ccccc12
Mol. weight [g/mol]:	179.22
CAS:	229-87-8

Physical Properties

Property code	Value	Unit	Source
chs	-6542.80 ± 1.20	kJ/mol	NIST Webbook
hf	240.50 ± 4.20	kJ/mol	NIST Webbook
hfs	141.90 ± 1.40	kJ/mol	NIST Webbook
hsub	98.60	kJ/mol	NIST Webbook
hsub	98.60	kJ/mol	NIST Webbook
hsub	98.60 ± 4.00	kJ/mol	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
ie	8.31 ± 0.02	eV	NIST Webbook
log10ws	-2.78		Estimated Solubility Method
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method
rinpol	307.94		NIST Webbook
rinpol	308.79		NIST Webbook
rinpol	306.30		NIST Webbook
rinpol	311.00		NIST Webbook
rinpol	307.03		NIST Webbook
rinpol	307.94		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1840.00		NIST Webbook

rinpol	1841.00		NIST Webbook
rinpol	308.10		NIST Webbook
rinpol	307.30		NIST Webbook
rinpol	308.27		NIST Webbook
rinpol	307.45		NIST Webbook
rinpol	307.30		NIST Webbook
rinpol	1840.00		NIST Webbook
ss	205.91	J/mol×K	NIST Webbook
ss	205.91	J/mol×K	NIST Webbook
ss	205.87	J/mol×K	NIST Webbook
tf	379.65 ± 1.00	K	NIST Webbook
tf	379.40 ± 1.00	K	NIST Webbook
tf	380.55	K	Aqueous Solubility Prediction Method
tf	377.00 ± 2.00	K	NIST Webbook
tf	372.65 ± 2.00	K	NIST Webbook
tf	379.65 ± 1.50	K	NIST Webbook
tt	379.10	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques
tt	379.94 ± 0.02	K	NIST Webbook
tt	379.74 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	201.87	J/mol×K	298.15	NIST Webbook
cps	201.79	J/mol×K	298.15	NIST Webbook
cps	201.87	J/mol×K	298.15	NIST Webbook
hfust	0.02	kJ/mol	354.00	NIST Webbook
hfust	22.83	kJ/mol	379.70	NIST Webbook
hfust	22.83	kJ/mol	379.70	NIST Webbook
hsubt	95.00 ± 4.00	kJ/mol	305.50	NIST Webbook
hsubt	100.00 ± 10.00	kJ/mol	305.50	NIST Webbook
hvapt	68.90 ± 0.10	kJ/mol	428.00	NIST Webbook
hvapt	71.60 ± 0.10	kJ/mol	428.00	NIST Webbook
hvapt	74.30 ± 0.10	kJ/mol	428.00	NIST Webbook
sfust	0.06	J/mol×K	354.00	NIST Webbook
sfust	60.12	J/mol×K	379.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	622.20	K	103.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C229878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of three-ring aza-aromatics. 2. Experimental results for 1,10-phenanthroline, phenanthridine, and 7,8-benzoquinoline, and mutual consistency of experiments and computational methods:	https://www.doi.org/10.1016/j.jct.2009.11.011
Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by combustion calorimetry and theoretical techniques:	https://www.doi.org/10.1016/j.tca.2016.05.001
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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