Phenazine

Other names:	9,10-diazaanthracene
	Azophenylene
	Dibenzo-p-diazine
	Dibenzoparadiazine
	dibenzopyrazine
Inchi:	InChI=1S/C12H8N2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14-10/h1-8H
InchiKey:	PCNDJXKNXGMECE-UHFFFAOYSA-N
Formula:	C12H8N2
SMILES:	c1ccc2nc3ccccc3nc2c1
Mol. weight [g/mol]:	180.21
CAS:	92-82-0

Physical Properties

Property code	Value	Unit	Source
affp	938.40	kJ/mol	NIST Webbook
basg	908.30	kJ/mol	NIST Webbook
chs	-6106.70 ± 3.30	kJ/mol	NIST Webbook
chs	-6109.10 ± 1.70	kJ/mol	NIST Webbook
chs	-6112.80 ± 6.30	kJ/mol	NIST Webbook
chs	-6102.40 ± 1.20	kJ/mol	NIST Webbook
ea	1.31 ± 0.10	eV	NIST Webbook
hf	343.60 ± 2.80	kJ/mol	NIST Webbook
hf	328.80 ± 2.90	kJ/mol	NIST Webbook
hf	338.30 ± 3.40	kJ/mol	NIST Webbook
hfs	243.70 ± 2.30	kJ/mol	NIST Webbook
hfs	237.00 ± 2.00	kJ/mol	NIST Webbook
hfs	241.30 ± 3.40	kJ/mol	NIST Webbook
hfus	24.92	kJ/mol	Thermodynamic properties of three-ring aza-aromatics. 1. Experimental results for phenazine and acridine, and mutual validation of experiments and computational methods
ie	8.33 ± 0.02	eV	NIST Webbook
ie	8.44 ± 0.02	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
log10ws	-4.61		Crippen Method

logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
rinpol	294.37		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
ripol	2557.00		NIST Webbook
tf	444.00 ± 2.00	K	NIST Webbook
tf	451.00 ± 3.00	K	NIST Webbook
tt	446.40	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	234.30	J/mol×K	298.15	NIST Webbook
hfust	18.88	kJ/mol	447.89	NIST Webbook
hfust	18.88	kJ/mol	447.89	NIST Webbook
hfust	24.92	kJ/mol	447.90	NIST Webbook
hfust	20.92	kJ/mol	450.20	NIST Webbook
hfust	20.92	kJ/mol	450.20	NIST Webbook
hsubt	92.70 ± 0.40	kJ/mol	354.00	NIST Webbook
hsubt	94.30 ± 0.40	kJ/mol	354.00	NIST Webbook
hsubt	96.97	kJ/mol	298.15	NIST Webbook
hsubt	92.40	kJ/mol	299.00	NIST Webbook
hsubt	90.00 ± 2.00	kJ/mol	281.20	NIST Webbook
hsubt	90.40 ± 1.70	kJ/mol	287.00	NIST Webbook
hvapt	76.70	kJ/mol	298.00	Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography
hvapt	66.10 ± 0.10	kJ/mol	450.00	NIST Webbook
hvapt	65.50 ± 0.10	kJ/mol	460.00	NIST Webbook
hvapt	65.00 ± 0.10	kJ/mol	470.00	NIST Webbook

Sources

Thermodynamic properties of three-ring aza-aromatics. 1. Experimental results for phenazine and acridine, and mutual validation of values	https://www.doi.org/10.1016/j.jct.2009.11.010
Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by Study of the Anomalous Experiments and Computational Methods	https://www.doi.org/10.1016/j.tca.2016.05.001
Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography: Method	https://www.doi.org/10.1021/je900702t
Fusion	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature