Quinoxaline

Other names:	1,4-Diazanaphthalene
	1,4-Naphthyridine
	1,4-benzodiazine
	Benzo[a]pyrazine
	Benzoparadiazine
	Benzopyrazine
	Phenopiazine
	Phenpiazine
	Quinazine
	USAF EK-7094
Inchi:	InChI=1S/C8H6N2/c1-2-4-8-7(3-1)9-5-6-10-8/h1-6H
InchiKey:	XSCHRSMBECNVNS-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1ccc2nccnc2c1
Mol. weight [g/mol]:	130.15
CAS:	91-19-0

Physical Properties

Property code	Value	Unit	Source
affp	903.80	kJ/mol	NIST Webbook
basg	873.70	kJ/mol	NIST Webbook
chs	-4179.30 ± 2.40	kJ/mol	NIST Webbook
ea	0.71 ± 0.10	eV	NIST Webbook
hf	240.30 ± 3.30	kJ/mol	NIST Webbook
hfs	173.70 ± 2.60	kJ/mol	NIST Webbook
hsub	66.60 ± 2.00	kJ/mol	NIST Webbook
hsub	69.40 ± 0.60	kJ/mol	NIST Webbook
hsub	66.60 ± 2.00	kJ/mol	NIST Webbook
hsub	66.60	kJ/mol	NIST Webbook
ie	8.99	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.02 ± 0.01	eV	NIST Webbook
ie	9.01 ± 0.01	eV	NIST Webbook
ie	9.01	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method

rinpol	220.37		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1905.00		NIST Webbook
tb	502.70	K	NIST Webbook
tb	494.70	K	NIST Webbook
tf	306.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	11.80	kJ/mol	305.70	NIST Webbook
hfust	11.80	kJ/mol	305.70	NIST Webbook
hsubt	69.39	kJ/mol	298.15	NIST Webbook
hvapt	58.70	kJ/mol	298.00	Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography:	https://www.doi.org/10.1021/je900702t
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91190&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
ea:	Electron affinity

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point