Pyridazine

Other names:	1,2-Diazabenzene
	1,2-Diazine
	Orthodiazine
Inchi:	InChI=1S/C4H4N2/c1-2-4-6-5-3-1/h1-4H
InchiKey:	PBMFSQRYOILNGV-UHFFFAOYSA-N
Formula:	C4H4N2
SMILES:	c1ccnnc1
Mol. weight [g/mol]:	80.09
CAS:	289-80-5

Physical Properties

Property code	Value	Unit	Source
affp	907.20	kJ/mol	NIST Webbook
basg	877.10	kJ/mol	NIST Webbook
chl	-2370.60 ± 0.92	kJ/mol	NIST Webbook
ea	0.01	eV	NIST Webbook
ea	-0.32	eV	NIST Webbook
hf	278.40 ± 1.30	kJ/mol	NIST Webbook
hfl	224.90 ± 0.92	kJ/mol	NIST Webbook
hvap	53.50	kJ/mol	NIST Webbook
hvap	53.50 ± 0.40	kJ/mol	NIST Webbook
hvap	53.50 ± 0.40	kJ/mol	NIST Webbook
ie	8.71 ± 0.00	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.71 ± 0.01	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.74 ± 0.11	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
log10ws	1.10		Aqueous Solubility Prediction Method
log10ws	1.10		Estimated Solubility Method
logp	0.477		Crippen Method
mcvol	63.420	ml/mol	McGowan Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	894.00		NIST Webbook

rinpol	894.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	480.35 ± 0.60	K	NIST Webbook
tb	481.20	K	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C289805&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
ea: Electron affinity
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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
tb: Normal Boiling Point Temperature