1,3-Diazine

Other names:	1,3-Diazabenzene
	Metadiazine
	Miazine
	Py
	Pyr
	Pyrimidine
	m-Diazine
Inchi:	InChI=1S/C4H4N2/c1-2-5-4-6-3-1/h1-4H
InchiKey:	CZPWVGJYEJSRLH-UHFFFAOYSA-N
Formula:	C4H4N2
SMILES:	c1cncnc1
Mol. weight [g/mol]:	80.09
CAS:	289-95-2

Physical Properties

Property code	Value	Unit	Source
affp	885.80	kJ/mol	NIST Webbook
basg	855.70	kJ/mol	NIST Webbook
chl	-2292.30 ± 0.84	kJ/mol	NIST Webbook
chl	-2288.90 ± 1.80	kJ/mol	NIST Webbook
ea	-0.25	eV	NIST Webbook
hf	195.80 ± 1.50	kJ/mol	NIST Webbook
hf	195.90 ± 1.40	kJ/mol	NIST Webbook
hfl	146.60 ± 0.84	kJ/mol	NIST Webbook
hfl	143.20 ± 1.80	kJ/mol	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
ie	9.73	eV	NIST Webbook
ie	9.73 ± 0.03	eV	NIST Webbook
ie	9.35 ± 0.01	eV	NIST Webbook
ie	9.42	eV	NIST Webbook
ie	9.32 ± 0.01	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.33 ± 0.07	eV	NIST Webbook
log10ws	1.10		Estimated Solubility Method

log10ws	1.10		Aqueous Solubility Prediction Method
logp	0.477		Crippen Method
mcvol	63.420	ml/mol	McGowan Method
rinpol	718.40		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	718.40		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	728.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1318.00		NIST Webbook
tb	396.70	K	NIST Webbook
tf	294.48	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C289952&Units=SI

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

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