Quindoxin

Other names:	Quinoxaline, 1,4-dioxide
	Bayo N-Ox
	BAY-Va 9391
	Celbar
	Grofas
	ICI 8173
	Quinoxaline di-N-oxide
	Quinoxaline dioxide
	Quinoxaline 1,4-di-N-oxide
	USAF H-1
	Chindoxin
	Chinoxalin-1,4-dioxid
	NSC 193508
	NSC 21653
Inchi:	InChI=1S/C8H6N2O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H
InchiKey:	CKIHZSGJPSDCNC-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	[O-][n+]1cc[n+]([O-])c2ccccc21
Mol. weight [g/mol]:	162.15
CAS:	2423-66-7

Physical Properties

Property code	Value	Unit	Source
chs	-4120.70 ± 0.90	kJ/mol	NIST Webbook
hf	227.10 ± 2.40	kJ/mol	NIST Webbook
hfs	115.10 ± 1.40	kJ/mol	NIST Webbook
hsub	112.00 ± 1.90	kJ/mol	NIST Webbook
hsub	112.00 ± 1.90	kJ/mol	NIST Webbook
ie	7.98 ± 0.05	eV	NIST Webbook
log10ws	-6.33		Crippen Method
logp	0.107		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2423667&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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