Pyrazine, 1,4-dioxide

Other names:	Pyrazine di-N-oxide
	Pyrazine dioxide
	Pyrazine N,N'-dioxide
Inchi:	InChI=1S/C4H4N2O2/c7-5-1-2-6(8)4-3-5/h1-4H
InchiKey:	SXTKIFFXFIDYJF-UHFFFAOYSA-N
Formula:	C4H4N2O2
SMILES:	[O-][n+]1cc[n+]([O-])cc1
Mol. weight [g/mol]:	112.09
CAS:	2423-84-9

Physical Properties

Property code	Value	Unit	Source
chs	-2215.30 ± 1.60	kJ/mol	NIST Webbook
hf	186.50 ± 1.90	kJ/mol	NIST Webbook
hfs	116.90 ± 0.80	kJ/mol	NIST Webbook
hsub	69.60 ± 1.70	kJ/mol	NIST Webbook
hsub	116.90 ± 0.80	kJ/mol	NIST Webbook
ie	8.33 ± 0.02	eV	NIST Webbook
log10ws	-4.53		Crippen Method
logp	-1.047		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
tf	574.00 ± 4.00	K	NIST Webbook

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=C2423849&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
tf:	Normal melting (fusion) point