2-Methylquinoxaline-1,4-dioxide

Other names: Quinoxaline, 2-methyl-, 1,4-dioxide
Inchi: InChI=1S/C9H8N2O2/c1-7-6-10(12)8-4-2-3-5-9(8)11(7)13/h2-6H,1H3
InchiKey: PZUHHXFIMAEXGO-UHFFFAOYSA-N
Formula: C9H8N2O2
SMILES: Cc1c[n+]([O-])c2ccccc2[n+]1[O-]
Mol. weight [g/mol]: 176.17
CAS: 6639-86-7

Physical Properties

Property code	Value	Unit	Source
chs	-4747.80 ± 3.40	kJ/mol	NIST Webbook
hf	169.90 ± 7.20	kJ/mol	NIST Webbook
hfs	62.90 ± 3.60	kJ/mol	NIST Webbook
hsub	107.00 ± 6.20	kJ/mol	NIST Webbook
hsub	107.00 ± 6.20	kJ/mol	NIST Webbook
log10ws	-6.81		Crippen Method
logp	0.415		Crippen Method
mcvol	126.150	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=C6639867&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume