Quinoxaline-2-carbonitrile, 3-amino-, 1,4-dioxide

Other names: 3-Amino-2-quinoxalinecarbonitrile 1,4-dioxide
Inchi: InChI=1S/C9H6N4O2/c10-5-8-9(11)13(15)7-4-2-1-3-6(7)12(8)14/h1-4H,11H2
InchiKey: ZGVCESZATUMTIM-UHFFFAOYSA-N
Formula: C9H6N4O2
SMILES: N#Cc1c(N)[n+]([O-])c2ccccc2[n+]1[O-]
Mol. weight [g/mol]: 202.17
CAS: 23190-84-3

Physical Properties

Property code	Value	Unit	Source
hsub	139.70 ± 3.70	kJ/mol	NIST Webbook
log10ws	-6.32		Crippen Method
logp	-0.440		Crippen Method
mcvol	137.510	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=C23190843&Units=SI

Legend

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