

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+][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/ci9903071
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

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