

2-Methyl-3-ethoxycarbonylquinoxaline, 1,4-dioxide

Other names:	3-Methyl-2-quinoxalinecarboxylic acid-1,4-dioxide, ethyl ester
Inchi:	InChI=1S/C12H12N2O4/c1-3-18-12(15)11-8(2)13(16)9-6-4-5-7-10(9)14(11)17/h4-7H,3H2
InchiKey:	GMGXWZSYCXQDEF-UHFFFAOYSA-N
Formula:	C12H12N2O4
SMILES:	CCOC(=O)c1c(C)[n+][[O-]]c2ccccc2[n+][O-]
Mol. weight [g/mol]:	248.23
CAS:	13297-18-2

Physical Properties

Property code	Value	Unit	Source
hsub	133.40 ± 2.10	kJ/mol	NIST Webbook
log10ws	-7.47		Crippen Method
logp	0.592		Crippen Method
mcvol	175.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13297182&Units=SI
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

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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