3-(Ethoxycarbonylmethylene)-2(1H)-quinoxalinon

Other names:	2-Quinoxalineacetic acid, 3,4-dihydro-3-oxo-, ethyl ester
	3-Hydroxy-2-quinoxalineacetic acid, ethyl ester
Inchi:	InChI=1S/C12H12N2O3/c1-2-17-11(15)7-10-12(16)14-9-6-4-3-5-8(9)13-10/h3-6H,2,7H2,
InchiKey:	PYZVMKLUEJUSEU-UHFFFAOYSA-N
Formula:	C12H12N2O3
SMILES:	CCOC(=O)Cc1nc2ccccc2[nH]c1=O
Mol. weight [g/mol]:	232.24
CAS:	14152-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	0.547		Crippen Method
mcvol	169.990	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=C14152568&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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