

3-Ethoxycarbonylquinoxaline 1-oxide

Inchi:	InChI=1S/C11H10N2O3/c1-2-16-11(14)9-7-13(15)10-6-4-3-5-8(10)12-9/h3-7H,2H2,1H3
InchiKey:	SFQPZXAGUSTDON-UHFFFAOYSA-N
Formula:	C11H10N2O3
SMILES:	CCOC(=O)c1c[n+][[O-]]c2ccccc2n1
Mol. weight [g/mol]:	218.21
CAS:	23395-75-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	1.045		Crippen Method
mcvol	155.900	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23395757&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

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

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