

2-Methyl-3-ethoxycarbonylquinoxaline,1-oxide

Other names:	3-(Methoxycarbonyl)-2-methylquinoxaline-1-oxide
Inchi:	InChI=1S/C12H12N2O3/c1-3-17-12(15)11-8(2)14(16)10-7-5-4-6-9(10)13-11/h4-7H,3H2,1
InchiKey:	VNYXIHXFVAWXAB-UHFFFAOYSA-N
Formula:	C12H12N2O3
SMILES:	CCOC(=O)c1nc2ccccc2[n+](O)c1C
Mol. weight [g/mol]:	232.24
CAS:	94098-94-9

Physical Properties

Property code	Value	Unit	Source
hsub	129.20 ± 4.10	kJ/mol	NIST Webbook
log10ws	-5.71		Crippen Method
logp	1.353		Crippen Method
mcvol	169.990	ml/mol	McGowan Method

Sources

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=C94098949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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