

2-Carbamoyl-3-methylquinoxaline

Other names:	3-methyl-2-quinoxalinecarboxamide
Inchi:	InChI=1S/C10H9N3O/c1-6-9(10(11)14)13-8-5-3-2-4-7(8)12-6/h2-5H,1H3,(H2,11,14)
InchiKey:	HIXVRVHZNVQVJS-UHFFFAOYSA-N
Formula:	C10H9N3O
SMILES:	Cc1nc2ccccc2nc1C(=N)O
Mol. weight [g/mol]:	187.20
CAS:	17357-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	1.822		Crippen Method
mcvol	140.050	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=C17357925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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