

[(3-Hydroxy-2-quinoxaliny)carbonyl] urea

Inchi:	InChI=1S/C10H8N4O3/c11-10(17)14-9(16)7-8(15)13-6-4-2-1-3-5(6)12-7/h1-4H,(H,13,15)
InchiKey:	QSCRRKZLIYRZAW-UHFFFAOYSA-N
Formula:	C10H8N4O3
SMILES:	NC(=O)NC(=O)c1nc2ccccc2nc1O
Mol. weight [g/mol]:	232.20
CAS:	6275-81-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	0.144		Crippen Method
mcvol	157.470	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6275816&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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