

Daniquidone

Other names:	Isoindolo(1,2-b)quinazolin-12(10H)-one, 8-amino-8-Aminoisoindolo[1,2-b]quinazolin-12(10H)-one
Inchi:	InChI=1S/C15H11N3O/c16-10-5-6-13-9(7-10)8-18-14(17-13)11-3-1-2-4-12(11)15(18)19/
InchiKey:	SRIOCKJKFXAKHK-UHFFFAOYSA-N
Formula:	C15H11N3O
SMILES:	<chem>Nc1ccc2c(c1)CN1C(=O)c3ccccc3C1=N2</chem>
Mol. weight [g/mol]:	249.27
CAS:	67199-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	2.317		Crippen Method
mcvol	180.180	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67199660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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