

4-Amino-2-chloro-6,7-dimethoxyquinazoline

Other names:	4-Quinazolinamine, 2-chloro-6,7-dimethoxy- 2-chloro-6,7-dimethoxyquinazolin-4-amine
Inchi:	InChI=1S/C10H10ClN3O2/c1-15-7-3-5-6(4-8(7)16-2)13-10(11)14-9(5)12/h3-4H,1-2H3,(H
InchiKey:	HWIIAAVGRHKSOJ-UHFFFAOYSA-N
Formula:	C10H10ClN3O2
SMILES:	COc1cc2nc(Cl)nc(N)c2cc1OC
Mol. weight [g/mol]:	239.66
CAS:	23680-84-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	1.883		Crippen Method
mcvol	162.460	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C23680844&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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