

2,4-Dichloro-6,7-dimethoxyquinazoline

Other names:	Quinazoline, 2,4-dichloro-6,7-dimethoxy-
Inchi:	InChI=1S/C10H8Cl2N2O2/c1-15-7-3-5-6(4-8(7)16-2)13-10(12)14-9(5)11/h3-4H,1-2H3
InchiKey:	DGHKCBSVAZXEPP-UHFFFAOYSA-N
Formula:	C10H8Cl2N2O2
SMILES:	COc1cc2nc(Cl)nc(Cl)c2cc1OC
Mol. weight [g/mol]:	259.09
CAS:	27631-29-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	2.954		Crippen Method
mcvol	164.720	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=C27631294&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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