2-Chloro-5-methoxybenzimidazole

Inchi: InChI=1S/C8H7ClN2O/c1-12-5-2-3-6-7(4-5)11-8(9)10-6/h2-4H,1H3,(H,10,11)
InchiKey: FMDGYQOERIOABX-UHFFFAOYSA-N
Formula: C8H7ClN2O
SMILES: COc1ccc2[nH]c(Cl)nc2c1
Mol. weight [g/mol]: 182.61
CAS: 15965-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	1.743		Crippen Method
mcvol	122.730	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=C15965545&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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