5-Chloro-2-methoxypyrimidine

Other names:	Pyrimidine,5-chloro-2-methoxy-
Inchi:	InChI=1S/C5H5ClN2O/c1-9-5-7-2-4(6)3-8-5/h2-3H,1H3
InchiKey:	GJNGJHZIOYFEOP-UHFFFAOYSA-N
Formula:	C5H5ClN2O
SMILES:	COc1ncc(Cl)cn1
Mol. weight [g/mol]:	144.56
CAS:	38373-44-3

Physical Properties

Property code	Value	Unit	Source
ie	9.36 ± 0.05	eV	NIST Webbook
log10ws	-1.81		Crippen Method
logp	1.139		Crippen Method
mcvol	95.620	ml/mol	McGowan Method

Sources

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=C38373443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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