

Imidazo[1,2-b]pyridazine,6-chloro-

Inchi: InChI=1S/C6H4ClN3/c7-5-1-2-6-8-3-4-10(6)9-5/h1-4H
InchiKey: MPZDNIJHHXRTIQ-UHFFFAOYSA-N
Formula: C6H4ClN3
SMILES: Clc1ccc2nccn2n1
Mol. weight [g/mol]: 153.57
CAS: 6775-78-6

Physical Properties

Property code	Value	Unit	Source
ie	8.55	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	1.383		Crippen Method
mcvol	98.660	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=C6775786&Units=SI>

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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<https://www.chemeo.com/cid/96-866-5/Imidazo-1-2-b-pyridazine-6-chloro.pdf>

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