1H-Imidazole-2-carboxaldehyde, 1-methyl-

Other names:	Imidazole-2-carboxaldehyde, 1-methyl- 1-Methyl-2-imidazolecarboxaldehyde
Inchi:	InChI=1S/C5H6N2O/c1-7-3-2-6-5(7)4-8/h2-4H,1H3
InchiKey:	UEBFLTZXUXZPJO-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	Cn1ccnc1C=O
Mol. weight [g/mol]:	110.11
CAS:	13750-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	0.233		Crippen Method
mcvol	83.380	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=C13750817&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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