

1H-Imidazole-2-carboxaldehyde

Other names:	Imidazole-2-carboxaldehyde 2-Formylimidazole 2-Imidazolecarboxaldehyde
Inchi:	InChI=1S/C4H4N2O/c7-3-4-5-1-2-6-4/h1-3H,(H,5,6)
InchiKey:	XYHKNCXZYYTLRG-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	O=Cc1ncc[nH]1
Mol. weight [g/mol]:	96.09
CAS:	10111-08-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	-0.260		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
rropol	1108.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10111087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rropol:	Non-polar retention indices

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