Quinoline-2-carboxaldehyde

Other names:	quinoline-2-carbaldehyde
Inchi:	InChI=1S/C10H7NO/c12-7-9-6-5-8-3-1-2-4-10(8)11-9/h1-7H
InchiKey:	WPYJKGWLDJECQD-UHFFFAOYSA-N
Formula:	C10H7NO
SMILES:	O=Cc1ccc2ccccc2n1
Mol. weight [g/mol]:	157.17
CAS:	5470-96-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.047		Crippen Method
mcvol	120.090	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=C5470962&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