4-Quinolinecarboxaldehyde

Other names:	Quinoline-4-carboxaldehyde
	Cinchoninaldehyde
	quinoline-4-carbaldehyde
Inchi:	InChI=1S/C10H7NO/c12-7-8-5-6-11-10-4-2-1-3-9(8)10/h1-7H
InchiKey:	MGCGJBXTNWUHQE-UHFFFAOYSA-N
Formula:	C10H7NO
SMILES:	O=Cc1ccnc2ccccc12
Mol. weight [g/mol]:	157.17
CAS:	4363-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.047		Crippen Method
mcvol	120.090	ml/mol	McGowan Method
rinpol	1494.20		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1494.20		NIST Webbook
rinpol	1526.00		NIST Webbook

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=C4363933&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices