1H-Indole-3-carboxaldehyde

Other names:	Indole-3-carboxaldehyde
	«beta»-Indolylaldehyde
	Indol-3-carboxaldehyde
	Indole-3-aldehyde
	Indole-3-carbaldehyde
	3-Formylindole
	3-Indolealdehyde
	3-Indolecarbaldehyde
	3-Indolecarboxaldehyde
	Indole-3-carboxyaldehyde
	beta-Indolylaldehyde
	1H-Indole-3-carbaldehyde
	Indol-3-carbaldehyde
	1H-Indole-3-aldehyde
	NSC 10118
Inchi:	InChI=1S/C9H7NO/c11-6-7-5-10-9-4-2-1-3-8(7)9/h1-6,10H
InchiKey:	OLNJUISKUQQNIM-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	O=Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	145.16
CAS:	487-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.498		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
rinpol	1816.10		NIST Webbook
rinpol	1816.10		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487898&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
rinpol:	Non-polar retention indices