

1H-Indole-3-carboxaldehyde, 7-methyl-

Other names:	3-Carboxaldehyde, 7-methylindole- 7-Methyl-1H-indole-3-carbaldehyde
Inchi:	InChI=1S/C10H9NO/c1-7-3-2-4-9-8(6-12)5-11-10(7)9/h2-6,11H,1H3
InchiKey:	KTUFZHVVBHKGKZ-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	<chem>Cc1cccc2c(C=O)c[nH]c12</chem>
Mol. weight [g/mol]:	159.18
CAS:	4771-50-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	1.807		Crippen Method
mcvol	124.390	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=C4771500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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