Indole-6-carboxaldehyde

Inchi: InChI=1S/C9H7NO/c11-6-7-1-2-8-3-4-10-9(8)5-7/h1-6,10H
InchiKey: VSPBWOAEHQDXRD-UHFFFAOYSA-N
Formula: C9H7NO
SMILES: O=Cc1ccc2cc[nH]c2c1
Mol. weight [g/mol]: 145.16
CAS: 1196-70-9

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	1743.50		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1196709&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.