

Indole-7-carboxaldehyde

Inchi: InChI=1S/C9H7NO/c11-6-8-3-1-2-7-4-5-10-9(7)8/h1-6,10H
InchiKey: XQVZDADGTFJAFM-UHFFFAOYSA-N
Formula: C9H7NO
SMILES: O=Cc1cccc2cc[nH]c12
Mol. weight [g/mol]: 145.16
CAS: 1074-88-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.498		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
rinpole	1424.90		NIST Webbook

Sources

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=C1074880&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/15-458-7/Indole-7-carboxaldehyde.pdf>

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