1-Indolinecarboxaldehyde, 6-nitro-

Inchi: InChI=1S/C9H8N2O3/c12-6-10-4-3-7-1-2-8(11(13)14)5-9(7)10/h1-2,5-6H,3-4H2
InchiKey: MHMYRSLSPGQNPB-UHFFFAOYSA-N
Formula: C9H8N2O3
SMILES: O=CN1CCc2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]: 192.17
CAS: 73816-58-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	1.114		Crippen Method
mcvol	132.020	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C73816587&Units=SI
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

Legend

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