1H-Indole, 1-acetyl-2,3-dihydro-6-nitro-

Other names: Indoline, 1-acetyl-6-nitro-
Inchi: InChI=1S/C10H10N2O3/c1-7(13)11-5-4-8-2-3-9(12(14)15)6-10(8)11/h2-3,6H,4-5H2,1H3
InchiKey: RLXSSISTKOLICZ-UHFFFAOYSA-N
Formula: C10H10N2O3
SMILES: CC(=O)N1CCc2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]: 206.20
CAS: 22949-08-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.504		Crippen Method
mcvol	146.110	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=C22949082&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