

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

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