6-Nitro-3-carbethoxy-1,2,7-trimethylindole

Inchi: InChI=1S/C14H16N2O4/c1-5-20-14(17)12-9(3)15(4)13-8(2)11(16(18)19)7-6-10(12)13/h6
InchiKey: SSYHHCUKTLJWLV-UHFFFAOYSA-N
Formula: C14H16N2O4
SMILES: CCOC(=O)c1c(C)n(C)c2c(C)c([N+](=O)[O-])ccc12
Mol. weight [g/mol]: 276.29
CAS: 52916-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.83		Crippen Method
logp	2.880		Crippen Method
mcvol	204.040	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52916060&Units=SI

Legend

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