

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

Inchi:	InChI=1S/C14H16N2O4/c1-5-20-14(17)11-9(3)15(4)13-8(2)6-7-10(12(11)13)16(18)19/h6
InchiKey:	OTGJOVPKDZGPDA-UHFFFAOYSA-N
Formula:	C14H16N2O4
SMILES:	CCOC(=O)c1c(C)n(C)c2c(C)ccc([N+](=O)[O-])c12
Mol. weight [g/mol]:	276.29
CAS:	52916-05-9

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:	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=C52916059&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

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