

Tropanyl indole-3-lactate

Inchi: InChI=1S/C19H24N2O3/c1-21-13-6-7-14(21)10-15(9-13)24-19(23)18(22)8-12-11-20-17-5
InchiKey: UWNZVZOXRZRTAJ-UHFFFAOYSA-N
Formula: C19H24N2O3
SMILES: CN1C2CCC1CC(OC(=O)C(O)Cc1c[nH]c3ccccc13)C2
Mol. weight [g/mol]: 328.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	1.758		Crippen Method
mcvol	251.200	ml/mol	McGowan Method
rinpol	3517.40		NIST Webbook
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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=U415032&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
rinpol: Non-polar retention indices

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