

[7-(Hydroxymethyl)-2,3,5,8-tetrahydro-1H-pyrrolizin-1-yl]-1H-pyrrole-3-carboxylate

InChI: C14H18N2O3
InChIKey: ZGASCOASXPMKAG-UHFFFAOYSA-N
Formula: C14H18N2O3
SMILES: COCC1=CCN2CCC(OC(=O)c3cc[nH]c3)C12
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	0.719		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook

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=R577932&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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