

N-formyltetrahydrocytisine

Inchi: InChI=1S/C12H18N2O2/c15-8-13-5-9-4-10(7-13)11-2-1-3-12(16)14(11)6-9/h8-11H,1-7H2
InchiKey: YCAYHACOUGYTQJ-UHFFFAOYSA-N
Formula: C12H18N2O2
SMILES: O=CN1CC2CC(C1)C1CCCC(=O)N1C2
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.85		Crippen Method
logp	0.476		Crippen Method
mcvol	170.460	ml/mol	McGowan Method
rinpole	2150.00		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=R320662&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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/18-729-3/N-formyltetrahydrocytisine.pdf>

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