

Methyl

1,1'-dimethyl-2-oxo-1',4a',5',5a',7',8',10',10a'-octahydrospiro-indoline-3-carboxamide

Inchi:	InChI=1S/C22H26N2O4/c1-13-15-11-24-9-8-22(17-6-4-5-7-18(17)23(2)21(22)26)19(24)1
InchiKey:	UTVSHFGLVLURNU-UHFFFAOYSA-N
Formula:	C22H26N2O4
SMILES:	<chem>COC(=O)C1=COC(C)C2CN3CCC4(C(=O)N(C)c5ccccc54)C3CC12</chem>
Mol. weight [g/mol]:	382.45
CAS:	13897-71-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.087		Crippen Method
mcvol	284.180	ml/mol	McGowan Method
rinpola	2942.00		NIST Webbook
rinpola	2942.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.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=C13897717&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemed.com/cid/118-873-2/Methyl-1-1-dimethyl-2-oxo-1-4a-5-5a-7-8-10-10a-octahydrospiro-indoline-3-carboxamide>

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