

1,3-Dimethyl-5-(3-oxocyclohexen-1-yl)hexahydro

Inchi:	InChI=1S/C12H14N2O4/c1-13-10(16)9(11(17)14(2)12(13)18)7-4-3-5-8(15)6-7/h6,9H,3-5
InchiKey:	UYQADBUJDKKEDO-UHFFFAOYSA-N
Formula:	C12H14N2O4
SMILES:	CN1C(=O)C(C2=CC(=O)CCC2)C(=O)N(C)C1=O
Mol. weight [g/mol]:	250.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.332		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R577685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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